Volume 1

Environmentally Preferable Options for Furniture Fire Safety

Low-Density Furniture Foam

DRAFT

www.epa.gov/dfe

EXECUTIVE SUMMARY

Issue

Efforts to improve the fire safety of furniture have protected property and saved lives. Fires involving ignitions of residential upholstered furniture constitute a leading cause of fire deaths and serious injuries associated with consumer products. According to the Consumer Product Safety Commission staff, the average annual fire losses for the years 1995-1999 were 460 deaths, 1,110 injuries and $130 million in property damage (CPSC Public Meeting, 2004). Flame retardants delay ignition and have proven to save lives. While benefits achieved through enhanced fire safety are critical, they should be achieved in a manner that minimizes risk to human health and the environment. The work summarized in this report arose from concern over potential human health and environmental impacts from the use of pentabromodiphenyl ether (pentaBDE). This chemical flame retardant is used in the manufacture of low-density, flexible polyurethane foam for upholstered furniture (residential, business and institutional), mattresses, bedding, carpet underlay and other articles. Studies around the world have found pentaBDE to be widespread in the environment and in human tissues. Recently the use of pentaBDE has been banned in the European Union and in Hawaii and California in the United States.

In late 2003, Great Lakes Chemical Corporation, presently the sole U.S. manufacturer of the commercial mixture known as pentaBDE, announced a voluntary phase-out of this chemical in the United States by December 31, 2004. This phase-out, along with anticipated implementation of more stringent national fire safety standards in residential upholstered furniture, has made the issue of finding alternatives to pentaBDE a critical priority for the furniture industry and all parties involved.

Partnership and Scope

EPA's Design for the Environment Program and Region IX have joined with a broad set of stakeholders to form the Furniture Flame Retardancy Partnership. Key players involved in the Partnership include members of the furniture industry, chemical manufacturers, environmental groups, the Consumer Product Safety Commission and the National Institute of Standards and Technology.

The Partnership is working to identify and assess environmentally safer alternatives to pentaBDE and to investigate other technologies for improving furniture fire safety. The primary purpose of this report is to provide up-to-date and objective information that will allow the furniture industry and chemical manufacturers to factor human health and environmental considerations into decision-making when identifying replacements for pentaBDE. The hazard, exposure and environmental assessment of chemical flame-retardant alternatives in this report is intended to be a first step in providing information that will serve as a basis for making decisions. Additional objectives of this report are to inform the reader of some considerations to take into account when selecting a replacement for pentaBDE and to introduce alternative technologies that may impact future methods of flame retarding furniture.

The Partnership recognizes that no single alternative is expected to provide an ideal solution to address every issue. Rather, the project members hope to identify the strengths of each alternative such that individual companies and consumers can make educated decisions that will best suit their needs.

Results

This report is the first product of the Furniture Flame Retardancy Partnership. To provide information for decision-making, the Partnership evaluated the leading chemical alternatives for flame retarding low-density flexible polyurethane foam. Four leading U.S. flame-retardant chemical manufacturers identified 14 chemical formulations that are potentially viable substitutes for pentaBDE in large-scale production of low-density flexible polyurethane foam. EPA assessed the hazards, potential exposures and tendency to bioaccumulate and persist in the environment for the chemicals in each formulation. Section 4 of this report is a summary of EPA's qualitative assessment, which is based on known or estimated effects on various toxicological and environmental endpoints. This section includes a summary chart (Table 4-1) with information on potential routes of exposure, based on physical and chemical properties. Section 4 also includes an explanation of how the information in the chart was developed.

Conclusions

This report summarizes the level of potential hazard associated with relevant endpoints. The information in Table 4-1 provides the best available information for making educated decisions about these alternative chemical products.

The Partnership plans to develop a process to identify additional toxicological data needed for adequately assessing the flame-retardant alternatives in Table 4-1. Industry will support this process and develop data to satisfy these needs over time, based on factors that include the market share achieved, production volumes and areas where predicted data indicates a moderate to high level of concern. Those flame-retardant products that emerge as the most popular replacement products for pentaBDE deserve this greater level of scrutiny based on their potential for exposure to humans and the environment during manufacture, use and disposal. The stakeholders in this Partnership will use this newly developed data (summarized in Table 4-1) to affirm short-term decisions. EPA has developed this alternatives assessment to serve as a potential model for addressing emerging chemical concerns.

Next Steps

In the future, the Partnership intends to evaluate additional chemical flame retardants that may be necessary to meet planned national fire safety standards. The Partnership would also like to develop a furniture design challenge to encourage the safest means (new designs, chemicals and materials) to meet furniture fire safety standards. Finally, the Partnership would like to stimulate innovation by providing EPA recognition for next-generation, safer chemical flame retardants and safer non-chemical technologies.

Updated information on the Furniture Flame Retardant Partnership will be available on EPA's Design for the Environment website: http://www.epa.gov/dfe/.

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LIST OF ACRONYMS

ADDpot	Potential Average Daily Dose
ADRpot	Potential Acute Dose Rate
AFMA	American Furniture Manufacturers Association
AFSC	American Fire Safety Council
AHFA	American Home Furnishings Alliance
APP	Ammonium Polyphosphate
ATSDR	Agency for Toxic Substances and Disease Registry
BCF	Bioconcentration Factor
BIFMA	The Business and Institutional Furniture Manufacturer’s Association
BFR	Brominated Flame Retardant
CBI	Confidential Business Information
ChV	Chronic Value
CCRIS	Chemical Carcinogenesis Research Information System
CIS	Chemical Information Systems
COC	Concentration of Concern
CPA	Clean Production Action
CPSC	Consumer Product Safety Commission
DART	Developmental and Reproductive Toxicology
DecaBDE	Decabromodiphenyl Ether
DfE	Design for the Environment
ECDB	Existing Chemicals Database
ECOSAR	Ecological Structure Activity Relationships
EFED	Environmental Fate and Effects Division
ELISA	Enzyme-Linked Immunosorbent Assay
EMIC	Environmental Mutagen Information Center
EPA	Environmental Protection Agency
EPIWIN	Estimations Program Interface for Windows
ETIC	Environmental Teratology Information Center
EU	European Union
FDA	Food and Drug Administration
GIF	Graphite Impregnated Foam
HLC	Henry’s Law Constant
HMTC	Hazardous Materials Technical Center
HPV	High Production Volume Chemicals
HSDB	Hazardous Substances Data Bank
IARC	International Agency for Research on Cancer
IRIS	Integrated Risk Information System
KI	Krueger International, Inc.
K_{oc}	Soil Adsorption Coefficient
K_{ow}	Octanol-Water Partition Coefficient
LADDpot	Lifetime Average Daily Dose
LOAEC	Lowest Observable Adverse Effect Concentration
LOAEL	Lowest-Observed Adverse-Effect-Level
MA TURI	Massachusetts Toxics Use Reduction
MDI	Methyl Diphenyl Diisocyanate

MOE	Margin of Exposure
NIOSH	National Institute for Occupational Safety and Health
NIST	National Institute of Standards and Technology
NOAEC	No Observable Adverse Effect Concentration
NOAEL	No-Observed Adverse-Effect-Level
NTE	Neurotoxic Esterase
NTP	National Toxicology Program
OctaBDE	Octabromodiphenyl Ether
OECD	Organization for Economic Cooperation and Development
OPPT	Office of Pollution Prevention and Toxics
PBDE	Polybrominated Diphenyl Ether
PEC	Predicted Environmental Concentration
PentaBDE	Pentabromodiphenyl Ether
PESTAB	Pesticides Abstracts
PFC	Plaque-Forming Cell
PPBIB	Poisonous Plants Bibliography
SIC	Standard Industrial Classification
SNUR	Significant New Use Rule
SWC	Surface Water Concentration
TCPP	Tris (chloropropyl) Phosphate
TDCPP	Tris (1,3-dichloro-2-propyl) Phosphate
TDI	Toluene Diisocyanate
TSCA	Toxic Substances Control Act
TSCATS	Toxic Substances Control Act Test Submissions
UFAC	Upholstered Furniture Action Council
USGS	U.S. Geological Survey
VCCEP	Voluntary Children's Chemical Evaluation Program

ABOUT THE PARTNERSHIP

U.S. EPA's Design for the Environment (DfE) Program is a results-oriented voluntary partnership program. It achieves risk reduction through pollution prevention and applying Agency expertise and technical tools.

Designing for the environment is incorporating environmental considerations into business decision making. The EPA DfE Program collaborates with industry sectors to help businesses design or redesign products, processes and management systems that are cleaner, more cost-effective and safer for the worker and the public.

The Furniture Flame Retardancy Partnership is a joint effort among the U.S. EPA DfE Program, U.S. EPA Region IX, all segments of the furniture industry supply chain, government and non-government groups to identify environmentally safer solutions for meeting current and future furniture fire safety requirements.

<u>Steering Committee Members</u>:

American Home Furnishings Alliance (AHFA) (formerly AFMA)
"AHFA understands and supports the long range nature of this project and encourages EPA to remain engaged with private sector stakeholders to develop environmentally sound solutions to fire safety."

Business and Institutional Furniture Manufacturer's Association (BIFMA) International
"BIFMA is committed to promoting sustainable work environments and business practices based on sound economics, environmental protection, and social responsibility."

American Fire Safety Council (AFSC)
"AFSC is committed to improving fire safety standards and saving lives...We expect this partnership to lead to the implementation of safe and environmentally sound approaches to fire safety."

GreenBlue
"GreenBlue is attracted to this partnership because of the rare opportunity to reconceive design criteria for flame-retardant products."

Partners:

FURNITURE MANUFACTURES

American Home Furnishings Alliance (AHFA) (formerly AFMA)

Business and Institutional Furniture Manufacturer's Association (BIFMA) International

Berkline/Benchcraft
Brayton International
Herman Miller
HNI Corporation (formerly Hon Industries)
Krueger International, Inc. (KI)
Steelcase

CHEMICAL MANUFACTURERS

American Fire Safety Council (AFSC)

Albemarle Corporation
Ameribrom, Inc. (ICL Industrial Products)
Great Lakes Chemical Corporation
Para Chem
Supresta (formerly Akzo Nobel)

FABRIC/BARRIER MANUFACTURERS

Craftex Mills
Culp
Felters
Glen Raven
Microfibres
National Textile Association
Quaker

NON-GOVERNMENTAL ORGANIZATIONS

Clean Production Action (CPA)
GreenBlue
Massachusetts Toxics Use Reduction Institute (MA TURI)

GOVERNMENTAL ORGANIZATIONS:

Consumer Product Safety Commission (CPSC)

National Institute of Standards and Technology (NIST)
Building and Fire Research Laboratory

1.0 INTRODUCTION

This volume contains the purpose and scope of the assessment, a description of the general characteristics of flame retardants, a general overview of exposure pathways and routes for flame retardants used in flexible polyurethane foam and the results of the assessments of 14 formulations of flame-retardant products most likely to replace commercially available pentabromodiphenyl ether (pentaBDE).

A second volume, subtitled, “Chemical Hazard Reviews,” consists of the complete data sets for each of the chemicals of the 14 formulations of flame-retardant products evaluated in this study. Volume 2 is available under a separate cover at http://www.epa.gov/dfe/.

1.1 Purpose of the PentaBDE Alternatives Analysis

A high volume of residential upholstered furniture sold in the United States contains low-density, flexible polyurethane foam. Without some form of fire protection, the foam is highly flammable. To address this safety issue, mandatory flammability standards and regulations have been enacted for residential upholstered furniture in California (California, Illinois, and Ohio have flammability standards for commercial furniture as well). The Upholstered Furniture Action Council (UFAC), an all-industry group, has also implemented voluntary standards for resistance to ignition from smoldering cigarettes. Most foam and furniture flammability standards and regulations (domestic and foreign) are performance based and do not specify particular chemicals or methods to achieve flame retardancy. Therefore, chemicals are not specifically required; rather, any method (chemical or product design) that achieves the standard is acceptable. Historically, halogenated flame-retardant chemicals, both brominated and chlorinated, have been used as a cost-effective method to meet standards without compromising product quality.

Polybrominated diphenyl ethers (PBDEs) make up a category of structurally similar chemical flame retardants, which are used in a variety of applications. The application of the individual PBDE varies according to the number and location of bromine atoms attached to the diphenyl ether. There are ten possible sites for bromine to bind; decabromodiphenyl ether representing full saturation. The structure for pentaBDE contains five bromine atoms ($C_{12}H_5Br_5O$). The bromine atoms can be bound to any of the carbon atoms, resulting in several possible isomers of pentaBDE (some of which are much more chemically stable than others). Figure 1-1 shows a generic figure for all PBDEs, where “m” and “n” refer to the number of bromine atoms bound to each aromatic ring. If $m + n = 5$, the resulting structure is a pentaBDE isomer.

Commercially available pentaBDE is actually a mixture of PBDE congeners where the primary component is pentaBDE. The remaining congeners typically include triBDE (0 to 1 percent), tetraBDE (24 to 38 percent), and hexaBDE (4 to 12 percent) (European Chemicals Bureau, 2001). For these congeners, $m + n = 3, 4,$ and 6 respectively. Unless otherwise noted, all references in this report refer to the commercial pentaBDE mixture rather than the pure pentaBDE chemical.

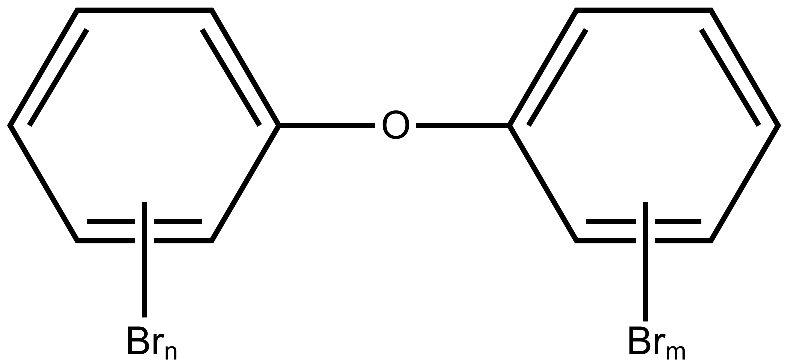

Figure 1-1 Pentabromodiphenyl Ether (pentaBDE), Where m+n = 5

Brominated flame retardants (BFRs), such as pentaBDE, act by chemical interaction to prevent the spread of a fire. Combustion is typically propagated by a series of chemical reactions, where oxygen combines with chemicals in the burning product. BFRs interrupt some of these reactions by volatilizing halogen radicals to react with the product in place of oxygen, slowing combustion.

PentaBDE has been the primary flame retardant for low-density, flexible polyurethane foam in residential furniture and mattresses for several years. About 8,500 metric tons of pentaBDE is used each year worldwide (Peltola and Ylä-Mononen, 2000) with approximately 98 percent of that being consumed in North America (Environ International Corp., 2003). Although pentaBDE saves lives by retarding fires, there is growing concern over the persistence and bioaccumulation of pentaBDE that may originate from foam manufactured with this chemical. More information on the presence of pentaBDE in the environment and biota, and its effects, can be found in Appendix A of this report. The European Union (EU) banned the use and sale of pentaBDE as of August 2004. Subsequently, the sole U.S. manufacturer of pentaBDE is conducting a voluntary phase-out of its production by December 31, 2004. In addition to the voluntary phase-out, legislation has been passed to prohibit the manufacturing, processing, or sale of substances or articles containing more than 0.1 percent by mass of pure pentaBDE in Hawaii and California in 2006 (January 1 and June 1, respectively).

The phase-out of production presents the need for alternatives to pentaBDE that are both environmentally safer and feasible for industry. In addition, the U.S. Consumer Product Safety Commission (CPSC) plans to implement new national fire safety standards regarding residential upholstered furniture that may lead to an increased need for flame-retardant furniture materials and an increased use of chemical flame retardants. The Furniture Flame Retardancy Partnership was formed as a result of this increased need to find practical alternatives that will suit the needs of all parties.

1.2 Scope of the PentaBDE Alternatives Analysis

Industry is actively exploring alternative methods to meet current and proposed fire safety standards. The Furniture Flame Retardancy Partnership is a project in which industry leaders have teamed with EPA and non-governmental environmental groups to evaluate each alternative based on human health, environmental, performance and cost considerations. The Furniture

Flame Retardancy Partnership will identify the characteristics of the alternatives and anticipates that industry will choose flame retardants that perform well in each of these areas as full-scale replacements for pentaBDE.

To date, the Furniture Flame Retardancy Partnership has evaluated available toxicological information for replacements for pentaBDE in low-density, flexible polyurethane foam. These are flame retardants that are viable options for meeting the performance requirements of California's TB117 standard. This report includes information prepared for this short-term goal and presents it in a common format that will be directly useful to industry as replacement flame retardants are selected.

The Furniture Flame Retardancy Partnership also has longer-term goals that are not included in this report. The next phase of this project will look at flame-retardant options for meeting the planned CPSC flammability standard for residential upholstered furniture. In the future, the Furniture Flame Retardancy Partnership intends to develop a process that will help industry to develop a common level of toxicological information for flexible foam flame retardants that attain a significant market share. The Partnership also intends to encourage development of safer flame retardants through high-level EPA recognition.

Alternative flame retardants can be separated into two categories: alternative chemicals and alternative technologies. The ideal chemical alternative would be a drop-in replacement that has similar physical and chemical properties to pentaDBE formulations such that existing storage and transfer equipment as well as foam production equipment can be used without significant modification. Most pentaBDE formulations are liquid, so most U.S. foaming operations are currently equipped to use liquid streams in the production of foam. Any chemical substitute that is not a liquid or is extremely viscous will require most U.S. operations to alter existing equipment – at significant cost – to accommodate the new chemical. If the alternative is not compatible with existing process equipment at foam manufacturing facilities, the plants will be forced to modify their processes and potentially have to purchase new equipment. Holding cost and feasibility as significant considerations, this report has focused on evaluating several of these potential drop-in chemicals.

Four chemical manufacturers have identified viable formulations for EPA review. These formulations are listed in Table 1-1. The chemicals in each formulation were screened for potential toxicological and environmental hazards as well as for potential exposure. A summary of the evaluations of this data is organized in Table 4-1 in Section 4.

The data presented on the formulations provide a means for comparison and allow the reader to conduct a screening-level hazard evaluation for each chemical alternative. Chemical release points and associated exposure routes and pathways for flame-retardant chemical manufacturing facilities, foam manufacturing facilities and furniture manufacturing facilities are included in Section 3 of this report.

Table 1-1 Potential Flame-Retardant Chemical Formulations

Albemarle Corporation	Ameribrom, Inc. (ICL Industrial Products)	Great Lakes Chemical Corporation	Supresta (Akzo Nobel)
SAYTEX® RX-8500	FR 513	Firemaster® 550	Fyrol® FR-2
SAYTEX® RZ-243		Firemaster® 552	AB053
ANTIBLAZE® 195			AC003
ANTIBLAZE® 205			AC073
ANTIBLAZE® 180			
ANTIBLAZE® V-500			
ANTIBLAZE® 182			

Non-chemical alternatives that eliminate the need for pentaBDE are addressed in Section 5.5 of this report. Though these technologies may not be considered feasible for immediate implementation or application for flame retarding foam, these alternative technologies are being considered for further investigation by the Furniture Flame Retardancy Partnership. Three currently-available, alternative technologies for flame retarding furniture include barrier technologies, graphite impregnated foam and surface treatment. There is considerable interest in future applications of these technologies for the furniture industry.

This report is intended to provide information that will allow industry and other stakeholders to evaluate environmentally safer alternatives for flame retarding furniture. The report is organized as follows:

- *Section 1 (Introduction):* This section provides a background to the Furniture Flame Retardancy project including the purpose and scope of the Partnership and of this report.

- *Section 2 (Chemical Flame Retardants):* This section describes characteristics of the flame-retardant chemicals currently used in flexible polyurethane foam and the mechanisms by which they suppress fires.

- *Section 3 (Exposure):* This section provides a general discussion of exposure concerns that should be evaluated when conducting an environmental risk assessment and identifies exposure pathways and routes associated with flame-retardant chemicals used in furniture manufacturing.

- *Section 4 (Alternatives Evaluations):* This section contains EPA's exposure and hazard assessments on a chemical-specific and formulation-specific basis for the flame-retardant formulations being evaluated.

- *Section 5 (Considerations):* This section addresses considerations for selecting a replacement for pentaBDE based on environmental and economic feasibility. It also includes alternative technologies that may serve as alternatives to chemical flame retardants.

2.0 TYPES OF CHEMICAL FLAME RETARDANTS

Publicly available scientific literature contains a wealth of information about various mechanisms of flame retardancy and characteristics of flame retardants. This section summarizes the general characteristics associated with flame retardants and associated mechanisms of flame retardancy.

2.1 General Characteristics of Chemical Flame Retardants

Some general characteristics of flame-retardant chemicals mandate how they interact with and flame retard the substrate in which they are used. This section defines some of these important characteristics, including:

- General mechanisms of flame retardancy;
- Additive and reactive flame-retardant chemicals; and
- Flame-retardant synergists.

2.1.1 General Mechanisms of Flame Retardancy

In general, flame retardants act in one of two ways; either by preventing ignition or preventing the spread of a fire. First, the ignition susceptibility of a product lowers when the flame retardant increases the net heat capacity of the product. Second, once a fire has already begun, flame retardants can reduce the tendency of the fire to spread by reacting with the product and forming a less flammable char or noncombustible gaseous layer along the boundary of the fire.

Within these two general flame-retardant mechanisms, Kirk-Othmer's Encyclopedia of Chemical Technology (Kirk-Othmer, 2001) provides a more detailed summary of five specific mechanisms by which flame retardancy may occur: physical dilution, chemical interaction, inert gas dilution, thermal quenching and protective coatings.

- **Physical dilution:** The flame retardant can act as a thermal sink, increasing the heat capacity of the product or reducing the fuel content to a level below the lower limit of flammability. Inert fillers such as glass fibers and microspheres and minerals such as talc act by this mechanism.

- **Chemical interaction:** The flame retardant dissociates into radical species that compete with chain propagating and branching steps in the combustion process. This is the general flame-retarding mechanism by which brominated flame retardants operate.

- **Inert gas dilution:** Flame-retardant additives produce large volumes of noncombustible gases when the product decomposes during combustion. The gases dilute the oxygen supply to the flame or dilute the fuel concentration below the flammability limit. Metal hydroxides, metal carbonates and some nitrogen producing compounds function in this way as flame retardants.

- **Thermal quenching:** Endothermic degradation of the flame retardant results in thermal quenching. Metal hydroxides and carbonates act in this way.

- **Protective coatings:** Some flame retardants function by forming a protective liquid or char barrier that acts as an insulating layer to reduce the heat transfer from the flame to the combusting product. Phosphorous compounds that decompose to give phosphoric acid and intumescent systems operate by this mechanism.

BFRs such as pentaBDE react chemically to prevent the spread of a fire. In products without BFRs, combustion is propagated by a series of chemical reactions that occur in the gas phase, where oxygen combines with chemicals in the burning product. BFRs interrupt some of these reactions by introducing the volatilized halogens to react with the product in place of oxygen, slowing combustion.

2.1.2 Additive and Reactive Flame Retardants

Flame retardants are categorized as either additive or reactive. Additive flame-retardant chemicals can be added to a manufactured product without bonding or reacting with the product. They are incorporated and dispersed evenly throughout the product, but are not chemically bound to it. Reactive flame-retardant chemicals may be incorporated into the product during manufacture of the plastic raw materials. They are chemically bound to the raw materials that are used to make the final product.

The basic mechanisms of flame retardancy (discussed earlier) will vary depending on the specific flame retardant and substrate. Additive and reactive flame-retardant chemicals can function in the vapor or condensed phase. Depending on the specific chemical, any of the mechanisms previously discussed may be utilized. Due to specific physical and chemical properties of the flame retardant and its effects on the substrate, most are used exclusively as either reactive or additive.

Additive Flame Retardants

Most flame retardants are used as additive flame retardants. Commercial pentaBDE is added at the time the polymer is formed. In general, additive flame retardants react when heated and either (a) emit substances that displace the oxygen needed for a fire to burn, (b) form a protective coating on the surface of a flammable substrate, thereby limiting access of the fire to fuel sources, or (c) do a combination of both. Halogenated flame retardants act in the gas phase by releasing chlorine- and/or bromine-containing radicals. In contrast, other flame retardants quench the flame by forming an intumescent, resinous char on the surface of the polymer. This char insulates and protects the polymer from further decomposition. The flame retardant in the system then expands, helping to form an insulating barrier that limits further damage to the polymeric material.

Additive flame retardants used in foam and other plastics are typically incorporated after manufacture of the polymer and during the manufacture of the end product (at the final product manufacturing facility). These additives are mixed into the polymer in common processing equipment concurrently with other ingredients such as stabilizers, pigments and processing aids. This is most likely to occur during a very preliminary stage at the end-product manufacturing facility (typically during the compounding step).

Reactive Flame Retardants

Reactive flame retardants are chemically bound to polymer products either by incorporating them into the polymer backbone during the polymerization reaction or by grafting them onto it. This is most likely to occur at the foam manufacturing facility. Therefore, reactive flame retardants are typically already incorporated in the raw materials that are purchased and received by the furniture manufacturers

Note that because they are chemically bound to the substrate, reactive flame retardants tend to exert a much greater effect than additive flame retardants on the properties of the polymer they are incorporated into.

2.1.3 Flame-Retardant Synergists

Many flame-retardant synergists do not have significant flame-retardant properties by themselves; however, their use increases the overall effectiveness of the flame-retardant system.

While char formation in the condensed phase and halogen interference in the vapor phase take place when flame retardants are used alone, the presence of a synergist can dramatically increase the flame retardant's effectiveness, lowering the quantity of the flame retardant needed to meet the required standard. Since high levels of flame retardants often affect product quality, a synergist to reduce the amount of flame retardant is often used. Additionally, the cost of flame retardants can be significant; therefore, any method to decrease the quantity of flame retardants needed is advantageous.

As an example of synergistic mechanisms, some synergists retard fire via two processes. In the condensed phase, a char layer is formed during the reaction with the synergistic compound, the flame retardant and the polymer. As discussed above, this char acts as a shield as it reduces the rate of decomposition of the polymer; therefore, less fuel is available for the flame. In the vapor phase, the chemical reaction is slowed down. This adds to the flame retardant's inhibitory effects on combustion by allowing it to react more completely with free radicals of oxygen and hydrogen, which are necessary for combustion to occur (Kirk Othmer, 2002).

As an example of how synergists can be used, consider organophosphorous flame retardants. When used alone, organophosphorous flame-retardant concentrations may need to be extremely high. These concentrations of the flame retardant often adversely affect the properties of the product. Testing has shown that adding inorganic synergists can dramatically increase the flame-retardant efficiency. Therefore, a significantly smaller quantity of the flame retardant is required. The synergistic effect on flame retardancy, coupled by the reduction in adverse effects on the product from the flame retardant is attractive to flame-retardant and end-product manufacturers.

2.2 Flame-Retardant Chemicals Currently Used in Foam

A wide variety of flame-retardant chemicals are currently in use throughout the world to meet fire safety standards for various types of foam. Many of these chemicals could theoretically be used to meet U.S. fire safety standards for low-density, flexible polyurethane foam. However, their use will result in trade offs. Some, for example require high loadings that result in an affect on foam quality. Others are cost prohibitive. Still others will require significant modifications in the handling and process equipment that is currently used in most U.S. foam manufacturing facilities. The environmental assessments presented in this report correspond to 14 specific formulations that chemical companies presented as the most viable large-scale substitutes for pentaBDE. However, other chemicals (besides these 14 formulations) are currently used for other types of foam and in niche markets for low-density polyurethane foam.

PentaBDE is an additive flame retardant that is used as a liquid formulation, typically blended with isopropylphenyl diphenyl phosphate/triphenyl phosphate and other additives. The commercial PentaBDE products are used to flame retard low-density, flexible polyurethane foam (Weil and Levchik, 2004). Great Lakes Chemical Corporation is the sole manufacturer of pentaBDE in the United States, but Ripplewood Phosphorus and Great Lakes produce pentaBDE flame-retardant products. PentaBDE composition in products is proprietary.

The remainder of this section briefly discusses three of the most commonly used chemicals that various reports have suggested may be viable alternatives to pentaBDE. The chemicals are used domestically and abroad to flame retard <u>high-density</u>, flexible polyurethane foam. Chemical companies and foam manufacturing facilities have experimented with their use in low-density flexible foams with moderate success. Generally the use of these chemicals either results in scorching of the foam (an aesthetic effect unless severe) or a negative effect on the physical properties of foam. Also, many formulations of these chemicals are available only as solids; making them less desirable as drop in substitutes for pentaBDE.

Melamine

There are numerous international manufacturers of melamine. Melamine and its derivatives are non-halogenated flame retardants, typically used as a crystalline powder. Flame retardants based on melamine are currently used in flexible polyurethane foams, intumescent coatings, polyamides and thermoplastic polyurethanes (Special Chemicals, 2004). They are used effectively in Europe in high-density flexible polyurethane foams but require 30 to 40 percent melamine per weight of the polyol.

Tris (1,3-dichloro-2-propyl) phosphate (TDCPP)

TDCPP is a chlorinated phosphate ester that is often used in polyurethane foam formulations. TDCPP comprises approximately 12 percent of the weight of the polyol in the final foam product (Weil and Levchik, 2004). It is used in high-density foam domestically and abroad and has been used domestically in low-density foams when light scorching (discoloration) is not a primary concern (Akzo Nobel, 2002). Note that TDCPP has been mistakenly referred to as tris (chloropropyl) phosphate (TCPP) in many reports.

Ammonium Polyphosphate (APP)

APP is an additive flame retardant containing nitrogen and phosphorus, typically used in a crystalline form. It is currently used to flame retard flexible and rigid polyurethane foams, as well as in intumescent laminations, molding resins, sealants and glues (Leisewitz et al., 2001). APP formulations comprise approximately 4 to 10 parts per hundred parts polyol in flexible foam, and 20 to 45 parts per hundred parts polyol in rigid foam.

APP is included in this section because it has been listed in multiple sources as a flame retardant for several products, including flexible, polyurethane foam. However, chemical manufactures and foam manufacturing trade groups do not consider it to be an alternative for pentaBDE on a large scale. Reasons for this are that APP is typically incorporated as a solid, it has adverse effects on foam properties and processing and it is not considered to be as effective as a fire retardant compared to other alternatives (U.S. EPA, 2002).

These chemicals have been used in the United States and around the world to flame retard flexible polyurethane foam. However, only pentaBDE is capable of achieving flame retardancy and non-scorching requirements in the low-density foam that is manufactured in the United States. While other flame retardants have historically been used and will continue to be used to flame retard higher-density foams, these flame retardants result in scorching in many low-density foam formulations. These chemicals are potential alternatives for pentaBDE, but scorching and other drawbacks must be addressed before large-scale use is feasible.

Scorching results in foam that has a color gradient but unless severe, it will not adversely affect flame retardancy or foam performance. White foam has become the industry standard for flame-retarded, low-density foam in the mattress and bedding industries, and in many upholstered furniture applications in the United States. The color of the foam, however, is not a determinant of its flame retardancy. Greater acceptance of darkened foams would allow manufacturers to choose from a wider variety of alternative flame retardants.

3.0 EXPOSURE TO FLAME-RETARDANT CHEMICALS IN FOAM

To evaluate the risk to human health and the environment that is associated with any of the alternatives to pentaBDE, many factors must be considered. Risk is a function of two parameters, hazard and exposure. If there is very little exposure, then even the most hazardous chemicals pose minimal risk. However, if exposure is not well characterized, it cannot be assumed that there is no risk. The purpose of this section is to identify the highest priority routes of exposure to flame retardant chemicals used in foam that need to be further assessed and quantified. This section should be considered with the chemical-specific hazard analysis presented in Section 4. This section provides: general background regarding exposure pathways, discusses factors that affect exposure potential in an industrial setting, provides process descriptions for the industrial operations involved in the furniture manufacturing supply chain (identifying the primary release points and exposure pathways) and discusses consumer and environmental exposures.

Exposures to specific chemicals are not discussed; rather, the purpose is to provide information such that the reader can identify and characterize potential exposures based on the physical and chemical properties of any pentaBDE alternative.

Exposure can occur at many points in the life cycle of a flame-retardant chemical. There is a potential for occupational exposures during industrial operations; exposure to consumers while the flame-retarded product is being used; and exposure to the general population and environment when releases occur from product disposal or from manufacturing facilities. Figure 3-1 presents a simplified life cycle for a flame-retardant chemical used in low-density polyurethane foam.

3.1 Exposure Pathways and Routes (General)

There are multiple ways people and the environment can be exposed to chemicals and the different types of exposures can impact the effect of the hazard. For instance, the toxicological effects from exposure to skin are different than those from exposures from swallowing or inhaling a chemical. Because of this, exposure is typically characterized by different *pathways* and *routes*.

An exposure pathway is the physical course a chemical takes from the source of release to the organism that is exposed (how the chemical gets to the individual). The exposure route is a description of how the chemical gets into the organism. The three primary routes of exposure are: inhalation, dermal absorption and ingestion.

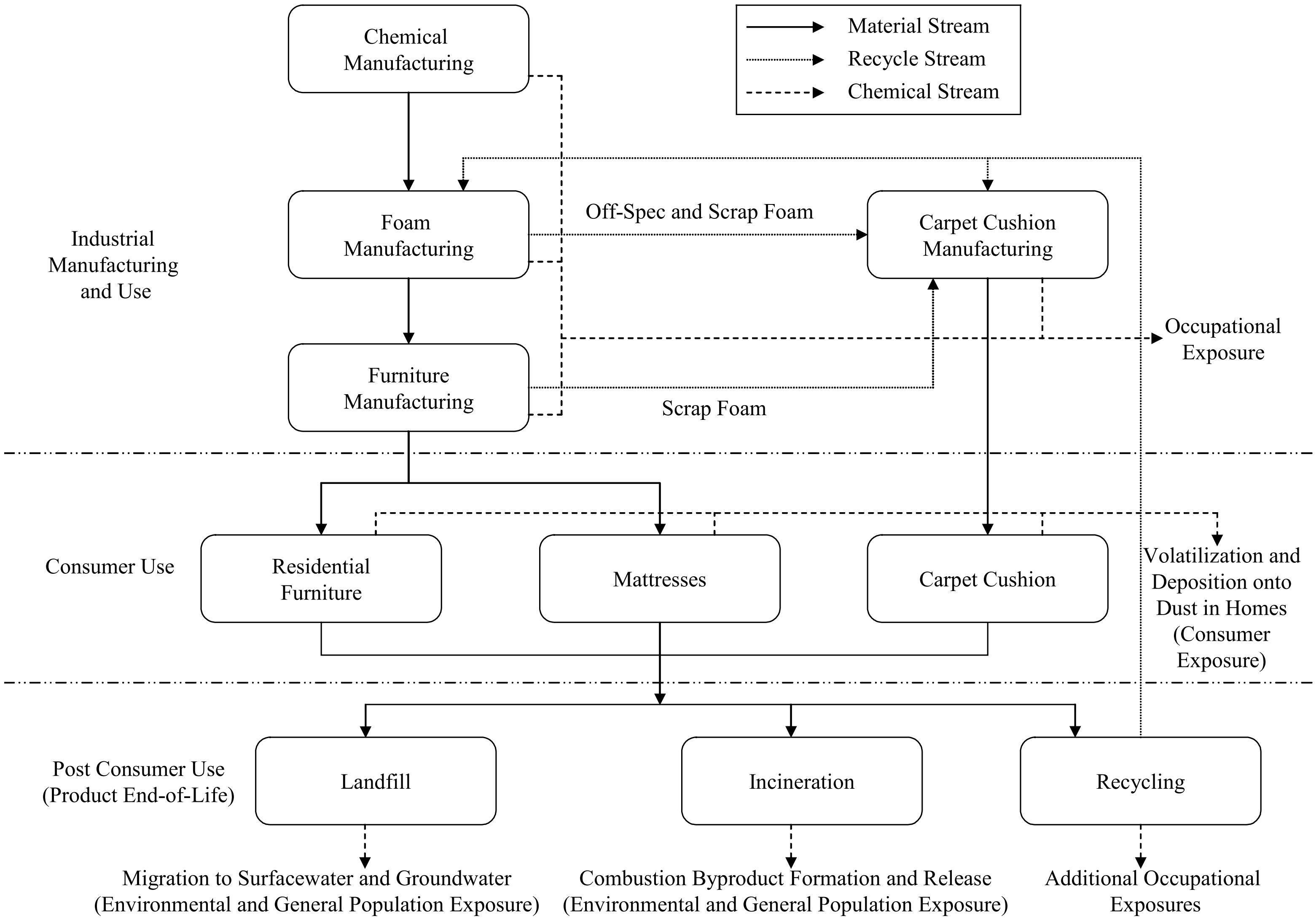

Figure 3-1 Simplified Life Cycle for a Flame-Retardant Chemical

Expected environmental releases and potential occupational exposures are dependent upon the physical and chemical properties of the chemical of concern. For example, a highly volatile liquid will readily evaporate from mix tanks and open transfer operations, potentially resulting in significant fugitive air releases and occupational exposures to workers that breathe the vapors. Conversely, chemicals that are manufactured and formulated as solids do not typically result in exposure to vapors, but may result in inhalation exposure to fugitive dust.

As noted above, risk is a function of the hazardous effects of an environmental toxicant and the level of exposure to it. Depending on the effects, exposure from only one or perhaps all three routes may result in significant risk. Therefore, each potential route should be evaluated independently along with an evaluation of appropriate endpoints. Endpoints are the specific toxicological effect, such as cancer, reproductive harm, organ/tissue damage or death.

There are circumstances when a chemical has serious effects for endpoint; however, its physical and chemical properties as well as environmental fate minimize the potential for it to be transported from the release point through the environment. This may essentially eliminate a potential pathway and route of exposure and eliminate the associated risk. For example, some chemicals are only hazardous if they are inhaled. If the chemical is non-volatile, the likelihood of breathing vapors containing the chemical is very low. This only generally applies to inhalation exposure from volatilization of liquid chemicals. If the chemical is solid, there is potential inhalation exposure associated with breathing dust. In another example, if the primary concern is due to skin sensitization, then a requirement for workers to wear appropriate gloves may reduce or mitigate the risk.

3.2 Industrial Releases and Exposures

This section provides process descriptions and identifies the corresponding release and exposure points for the unit operations that are involved within the furniture manufacturing supply chain. It should be noted that many of the potential occupational exposures identified here could be reduced or eliminated by the use of engineering controls and personal protective equipment. Also, some releases will only result in exposure to workers, while other releases result in exposures to the environment and the general population. The level of exposure between workers and the general population will vary considerably. Therefore, a risk evaluation should address occupational exposures separately from environmental and general population exposure.

Factors to consider when identifying and assessing potential pathways and routes of exposure are discussed below. Examples provided are occupational exposures. A more in-depth review of occupational exposures, consumer and general population exposures follows.

Inhalation Exposures

The physical state of the chemical during chemical manufacturing and downstream processing has a significant effect on the potential for inhalation exposure to workers. In particular, the physical state can result in three types of inhalation exposures that should be evaluated:

Dust: Chemicals that are manufactured, processed and used as solids have the potential to result in occupational exposure to fugitive dusts. The potential for significant dust formation depends on whether the solid chemical is handled in the crystalline form, as an amorphous solid, or a fine powder. Formation and handling of crystals and amorphous solids results in significantly less dust than powders. If there is exposure to dust, the level of exposure is directly proportional to the concentration of chemical in the particulate form. Therefore, a flame retardant that is used at a lower concentration results in a decreased exposure from this pathway and route (assuming an equivalent amount of dust is inhaled).

When assessing occupational exposures to pentaBDE alternatives, it is important to note the physical state of the chemical at the potential point of release and contact. The pure chemical may be manufactured as a solid powder, indicating a potential exposure to dust. However, it may be formulated into solution before any workers come in contact with it; thereby eliminating inhalation exposure to dust as a potential route.

Vapor: Exposure to vapors can occur when liquid chemicals evaporate during manufacturing, processing and use. Most chemical manufacturing operations occur in closed systems such that vapors are contained. However, fugitive emissions are expected during open mixing operations, transfer operations and loading/unloading of raw materials. More volatile chemicals evaporate more quickly and result in greater fugitive releases and higher occupational exposures than less volatile chemicals. Therefore, vapor pressure is the best indicator of potential occupational exposures to vapors. Studies have indicated that in some situations there is a potential for chemicals to volatilize from foam during the use of the consumer product (Wilford et al., 2003).

Mist: Non-volatile liquids can result in inhalation exposure if manufacturing or use operations result in the formation of mist. Therefore, risk assessors always address the potential for exposure from this pathway. It is unlikely that flame-retardant chemicals used as alternatives to pentaBDE on a large scale will be applied as a mist. However, some flame retardants that are applied as surface treatments can be spray applied. In these situations, exposure to mist will occur and should be evaluated.

Dermal Exposures

Occupational dermal exposure is also affected by the physical state of the chemical at the point of release and contact. For example, the likelihood of liquids being splashed or spilled during sampling and drumming operations is different than similar operations involving polymerized solids, powders, or pellets.

Dermal exposure is also generally assumed to be proportional to the concentration of chemical in the formulation. For instance, the dermal exposure from contacting a pure chemical is greater than the exposure from contacting a solution that contains only 10 percent of the chemical.

Screening-level evaluations of occupational dermal exposure can be based on the worker activities involving the chemical. For example, there may be significant exposure when workers handle bags of solid materials during loading and transfer operations. Maintenance and cleanup activities during shut down procedures, connecting transfer lines, and sampling activities also result in potential dermal exposures.

Ingestion

Occupational exposures via this route typically occur unintentionally when workers eat food or drink water that has become contaminated with chemicals. Two pathways should be considered. First, dust particles may spread throughout the facility and settle (or deposit) on tables, lunchroom surfaces, or even on food itself that is consumed. Vapors similarly spread throughout the facility and can adsorb into food and drinking water.

Another potential pathway for ingestion occurs from dust particles that are too large to be absorbed through the lungs. These “non-respirable particles” are often swallowed, resulting in exposures from this route.

While ingestion is considered to be a realistic route of exposure to workers, it is often considered less significant when compared to inhalation and dermal exposures, based on the relative exposure quantities. Ingestion during consumer use and to the general population is often as significant as or more important than the inhalation and dermal routes. If persistent and bioaccumulative compounds get into the environment and build up in the food chain, they can become a significant exposure concern.

The unit operations associated with each industry sector of the furniture supply chain result in a unique set of potential release points and occupational exposures to flame retardant chemicals. Sections 3.2.1 through 3.2.3 present an overview of typical manufacturing processes for these industry sectors. Potential release points and associated exposure concerns are noted, as appropriate.

3.2.1 Chemical Manufacturing

The specific unit operations, operating conditions, transfer procedures and packaging operations vary with the manufacture of different flame-retardant chemicals. The expected releases and occupational exposures depend on these parameters, the chemical’s physical state upon release and its physical and chemical properties. While it is outside the scope of this report to identify and quantify the releases and exposures associated with individual chemicals, this section presents a description of a typical chemical manufacturing process, identifies the potential releases and notes those that are most variable based on the flame-retardant chemicals produced. Figure 3-2 presents a generic chemical manufacturing process flow diagram and identifies the primary release and occupational exposure points.

The first step in most chemical manufacturing processes is to load or charge raw materials into some type of reactor or mix tank. Production volumes and batch sizes associated with flame-retardant chemicals typically require the raw materials to be stored in large tanks or drums until use. Large-quantity liquids are typically pumped into the reactor and solids are weighed and transferred via conveyorized, mechanical systems. Small-quantity raw materials may be manually introduced or carefully metered via automated systems. Releases and exposures are expected from these operations but they are associated with the raw materials, not the finished flame-retardant product.

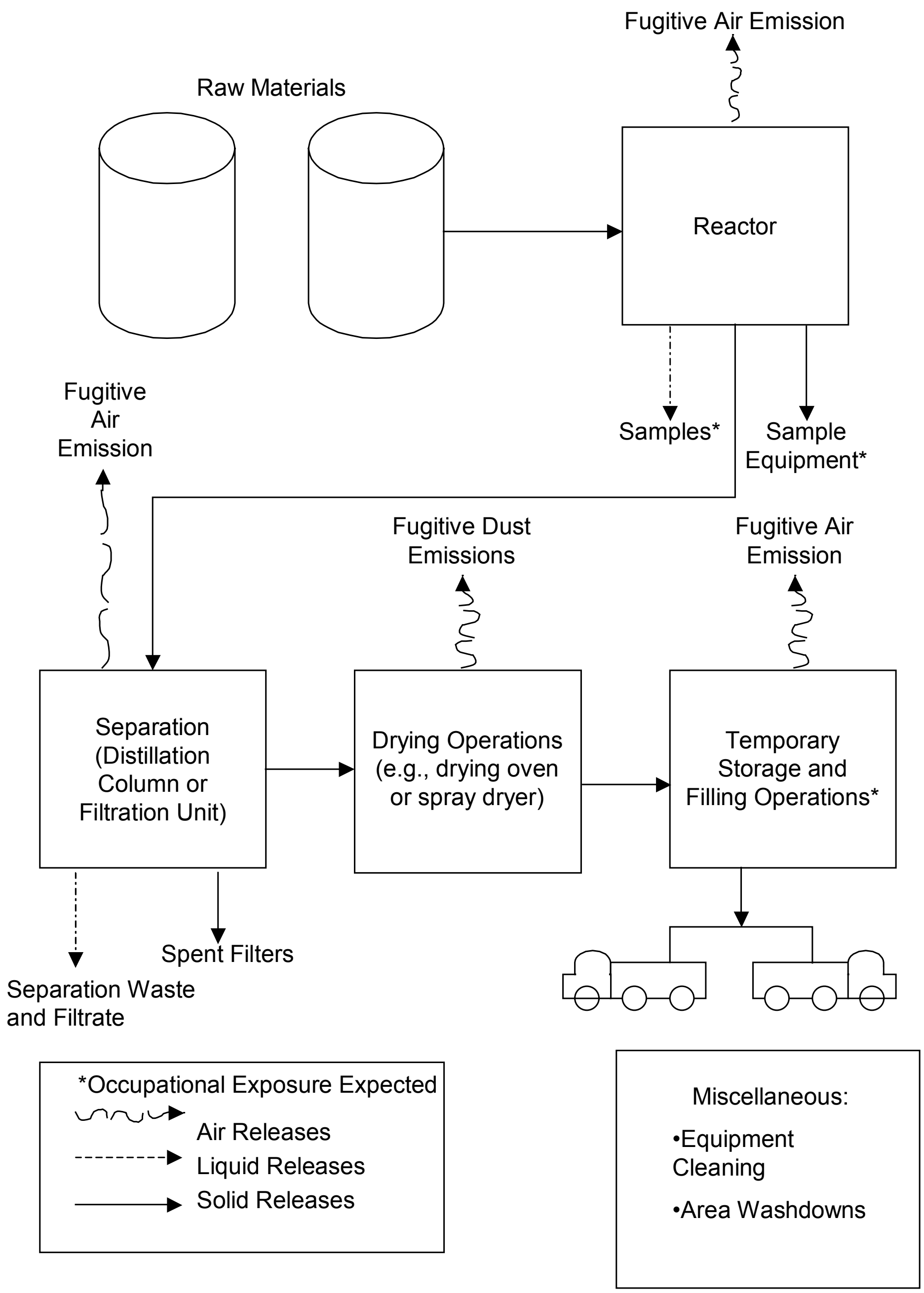

Figure 3-2 Generic Chemical Manufacturing Process Flow Diagram

Crude or intermediate products may be transferred through a series of reactors, distillation columns, filtration systems, drying ovens, spray dryers and other unit operations. These processes typically occur in closed systems, with engineering controls that serve both to regulate operating parameters such as temperature and pressure as well as to minimize fugitive releases. However, there is potential for a variety of solid and liquid releases from these operations, from cleaning process equipment and from sampling activity. Additionally, crude or finished products may be stored on-site in drums, day-tanks, or more permanent storage vessels until the flame-retardant formulation is packaged and shipped to customers (e.g., foam and textile manufacturers). The transfer and packaging operations are expected to result in releases of and exposures to the flame-retardant chemicals. Finally, miscellaneous operations, such as routine and unplanned maintenance activities, can result in considerable releases and exposures.

After the flame retardant is manufactured, it may need to be formulated into a solution, slurry, or mixture prior to introduction into the commercial flame-retardant formulation. For example, fine powders of a chemical may be formulated into an agglomerated powder or into a solution. The formulation steps usually occur at the chemical manufacturing facility, but additional mixing steps can occur at the foam manufacturing plant.

Release points from manufacturing and formulating can include:

- Transfer and packaging operations involving handling a chemical product;
- Routine and unplanned maintenance activities;
- Leaks from pumps and pipelines;
- Fugitive emissions from equipment;
- Product sampling; and
- Equipment and transport and storage vessel cleaning.

3.2.2 Foam Manufacturing

Flexible polyurethane foam is manufactured as slabstock foam or molded foam. The typical process used to manufacture each of these is described below. Rigid polyurethane foam is not discussed here because pentaBDE is used exclusively in flexible foam.

Slabstock Foam

The majority of flexible polyurethane foam is manufactured in slabstock operations. The slabstock manufacturing process is a continuous process that produces long, rectangular, continuous slabs of foam, called “buns”. Buns are cut into the desired configuration for an application, such as in furniture padding, bedding, automobile padding and seats, packaging materials and carpet padding.

The typical commercial process for slabstock foam production consists of a single unit operation, operated in batches. Figure 3-3 presents a generic diagram for this process. The raw materials include diisocyanates, polyol, water, auxiliary blowing agents, filler, chain modifying agents and other additives (including flame retardants).

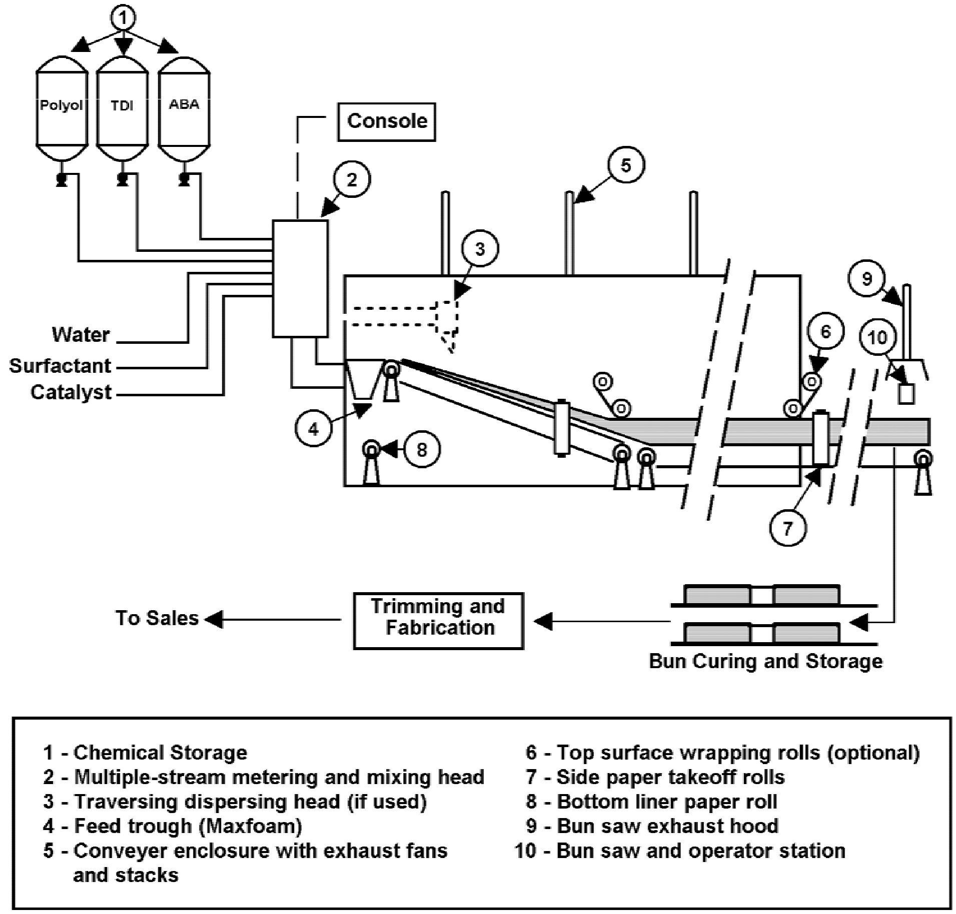

Figure 3-3 Typical Slabstock Foam Production for Flexible Polyurethane Foam

First, the raw materials and additives are metered into a single mix head, which dispenses the mixed materials to an enclosed conveyor system. Within a few minutes of leaving the mix head, the raw materials begin to create foam-producing reactions, producing the polyurethane foam on the conveyor. Most foam manufacturers have computerized controls at the mix head metering system that allow the raw materials mixture to be changed mechanically, without worker exposure to the chemicals.

The foam mixture moves down the conveyor at approximately 15 feet per minute. The conveyor is housed in a tunnel that is ventilated to remove the gases that are given off in the foam reaction. The foam reaches its full height of 2 to 4 feet in approximately 1 to 2 minutes. After 5 to 10 minutes, polymerization reactions are complete enough for the foam to be handled and cut. Workers typically enter the tunnel during startup and shutdown procedures or during upset conditions and usually wear appropriate personal protective equipment. Therefore, this potential occupational exposure point may be mitigated. Gases are often channeled away from the workplace and out the facility roof. Therefore, this is a potential environmental release point. The use of activated carbon filters or other organic vapor control devices on this stream can reduce releases from this exhaust stream.

A “flying saw” is often used to cut foam on the production line. This is an overhead saw that moves at the same rate as the conveyor while cutting the foam, in order to produce a straight cut. Each cut of foam is removed from the conveyor and moved to a curing area. Typically, buns are cured for 24 hours before further fabrication or shipping. Off gassing may occur during this step. Therefore, there is potential for inhalation exposure to volatile chemicals from curing operations.

Fabrication includes cutting and slicing the foam to meet the specifications of the customer. A machine called a slitter cuts large buns into a desired thickness. Vertical bandsaws or hand cutting are used to convert slabs of foam into smaller components for the desired end use (e.g., furniture). Dermal exposure and exposure to particulates may occur during this step.

Molded Foam

Molded flexible foam is produced when the foam polymerization reaction occurs in a closed mold resembling the final product. Molded foam is used in the transportation industry for seat cushions and interior trim, furniture, bedding, packaging materials, toys and novelty items.

The typical commercial process for molded foam production consists of a circular production line containing multiple molds and process stations. Figure 3-4 presents a diagram of this process.

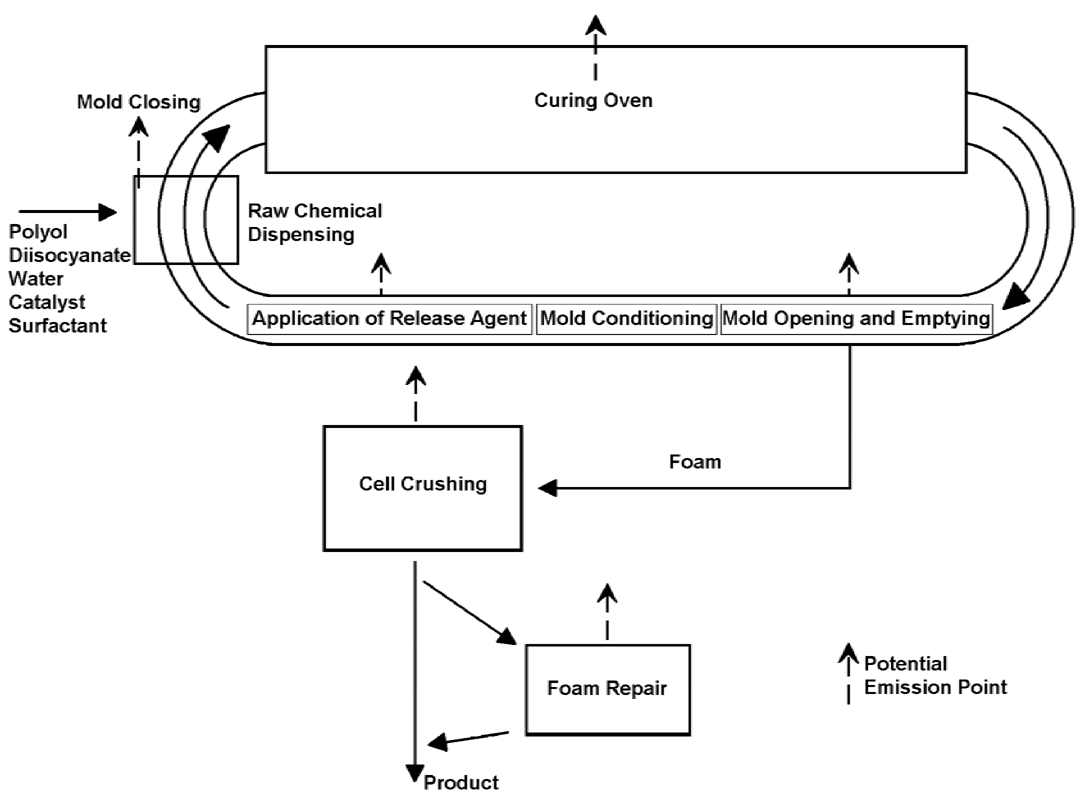

Figure 3-4 Typical Molded Foam Production Line for Flexible Polyurethane Foam

Raw materials include polyol, diisocyanates, water, catalyst, surfactant and other additives (e.g., flame-retardant formulation). The raw materials are pumped to a common mix head above the production line. Many ingredients are premixed to minimize the streams being fed to the head and to ensure precise measurement. The mix head dispenses a measured amount of the mixture into each mold and the molds are then heated to accelerate foam curing. Heating takes place either by passing the mold through a curing oven or passing heated water through tubes in the mold. Then, the mold is opened and emptied. The mold continues through the process line to be conditioned for the next product.

Primary release points and corresponding occupational exposures occur from fugitive emissions during transfer operations and opening/closing the molds. Additional releases and exposures occur from frequent equipment cleaning operations.

3.2.3 Furniture Manufacturing

Upholstered furniture manufacturers typically receive foam on site, and do not directly handle flame-retardant chemical formulations. The primary modes of exposure and releases are due to worker contact with the treated foam. Primary activities where exposure and releases may occur are during receipt of the foam, cutting and trimming and the placement on the furniture. Figure 3-5 presents a simplified process flow diagram for furniture manufacturing processes. A significant release may occur from flame-retarded scrap foam. Foam scrap from cutting and trimming operations is usually sold and utilized in the manufacture of carpet pad foaming. Otherwise the scrap is disposed of in landfills or by incineration.

Occupational Exposures

Occupational exposures during furniture manufacturing operations may occur due to inhalation of airborne fibers from handling operations and dust generated during cutting and dermal contact with treated foam. Workers will be directly exposed to foam that contains flame retardants on a regular basis as they handle the foam when it is received from suppliers, during incorporation into furniture and during cutting and cleanup activities.

Releases to Water

Furniture assembly is a dry process; therefore, there are no process water releases that are expected to contain flame retardants. Additionally, flame retardants are not expected to be formulated or applied at furniture manufacturing facilities unless the facility elects to use a post-manufacturing surface treatment alternative. Therefore, waste from container residue or equipment cleaning is not expected to contain flame retardants.

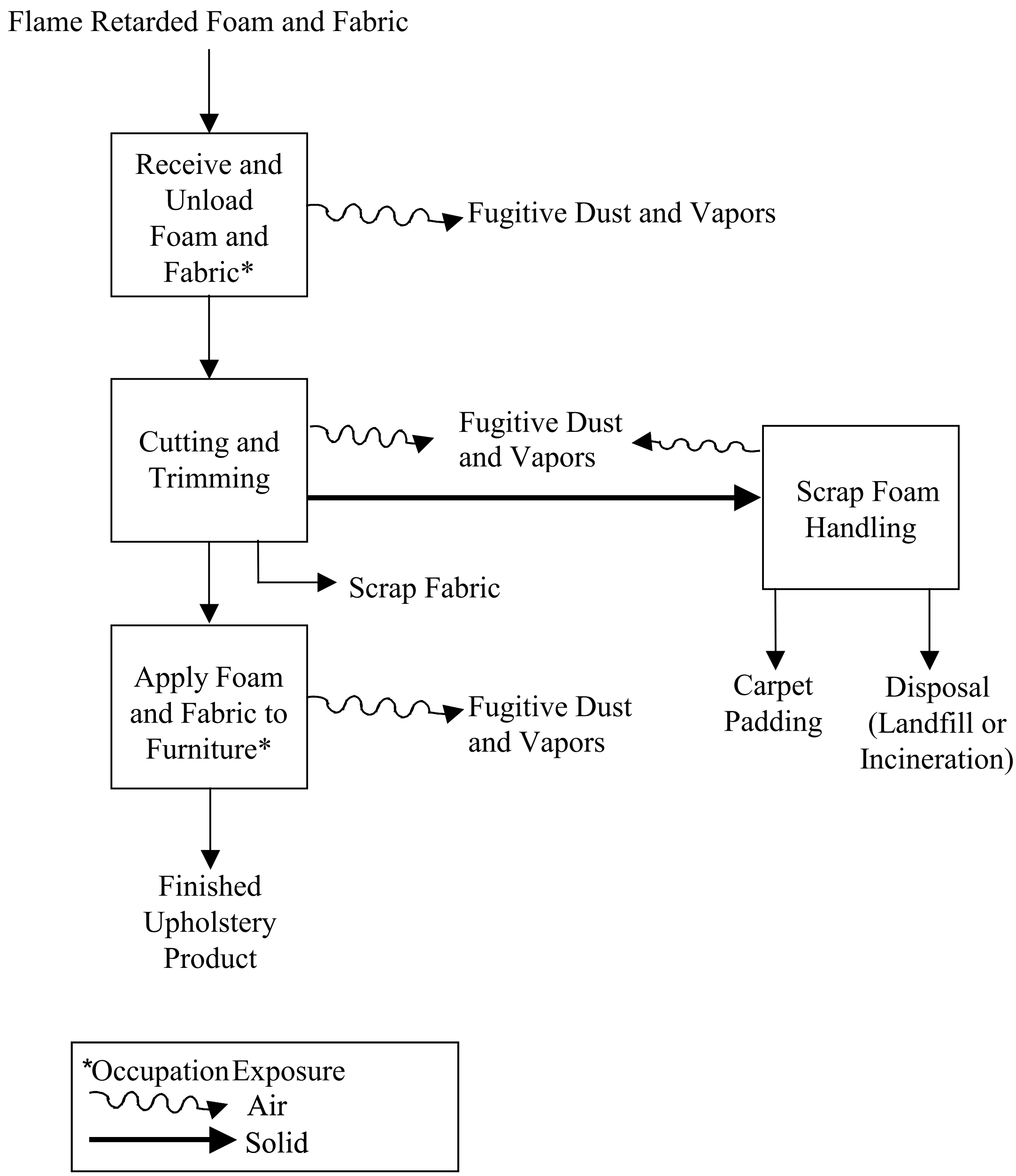

Figure 3-5 Process Flow Diagram: Furniture Manufacturing

Releases to Air

It is possible that dust or vapors will be generated and emitted as stack or fugitive emissions as a result of cutting operations during furniture assembly. Although some air emissions of fugitive dust containing flame retardants from the facility are possible, the quantity of dust generated and released to workplace and ambient environments has not been reported.

Releases to Land

The primary potential source of flame-retardant releases to land is scrap from cutting and trimming operations and floor sweepings. The foam from this waste source is typically collected and recycled in carpet cushion manufacturing, but may be sent to a landfill.

3.3 Consumer and General Population Exposures

Exposures to consumers and the environment are different from exposures to workers and should be evaluated separately for a number of reasons. Occupational exposures typically result from direct contact with chemicals at relatively high concentrations while workers are conducting specific tasks. Conversely, consumers may be exposed over a much longer period, but to a much smaller level because the chemical is incorporated into the product. Also, the general population and the environment will be exposed via different pathways and routes than workers and consumers. For example, a person that does not own a flame-retarded furniture product may still be exposed if the chemical leaches from the disposed product into the drinking water supply. Once in the water supply, groundwater, or surface water, it can be ingested by people or consumed by fish and other animals. Similarly, if the chemical is released to the atmosphere during manufacture, use or disposal, it may settle out on food crops and be ingested directly by people, or by cattle or other livestock. If the chemical is bioaccumulative, it may concentrate in the animal and reach people through the food chain. For these reasons, exposure to the environment and the general population should be assessed independently from occupational exposure.

A quantitative exposure assessment is outside the scope of this report. However, the primary pathways and routes from environmental, general population and consumer exposures are discussed in the following sections. Important chemical-specific factors that may help the reader compare exposure concerns between various pentaBDE alternatives are also discussed.

3.3.1 Physical and Chemical Properties Affecting Exposure

As previously discussed, the physical and chemical properties of a chemical often determine the potential (or at least the most likely) pathways and routes of exposure. In addition, the chemical properties dictate how the chemical will become distributed in the environment once it is released. These interactions in turn dictate the potential for the chemical to be transported from the release point to the receptor, and the availability for uptake into our bodies.

Additive vs. Reactive Chemicals

Regardless of the specific chemical composition, flame retardants are often categorized as either additive or reactive. Reactive flame retardants are chemically bound to the raw materials that are used to make the final product (i.e., bound to monomers and polymers that make up foam products). Additive flame retardants are incorporated and dispersed evenly throughout the foam, but are not chemically bound to it.

Depending on the product and its end use, additive flame retardants can eventually wash off (e.g., from textiles that are frequently cleaned), volatilize (e.g., from some plastic and foam), or leach from furniture after it has been disposed of in a landfill. This results in potential exposures to consumers, the environment and the general population because the furniture itself can be a source of release. Each furniture article may release very small amounts of the chemical over a period of several years. However, the combined effect of millions of articles may be very significant.

Reactive flame retardants are chemically bound to the foam either by incorporating them into the polymer backbone during the polymerization reaction or by grafting them onto it. This is most likely to occur at the foam manufacturing facility. Therefore, reactive flame retardants are typically already incorporated in the foam that is purchased and received by furniture manufacturers.

Because reactive flame retardants are chemically bound to the foam, it is far less likely they will be released. It should be noted that even reactive chemicals or close analogues can be released from the finished article; either when they are liberated from the polymer backbone or because some of the chemical was not completely reacted during the polymerization process. Also, note that because they are chemically bound to the substrate, reactive flame retardants tend to exert a much greater effect than additive flame retardants on the properties of the polymer they are incorporated into.

Properties Affecting Transport in the Environment (Vapor Pressure, Water Solubility)

If a chemical is released into the environment, either from the finished foam article or directly from an industrial facility, there still may not be significant exposures unless there is a potential for it to travel from the source to the receptor. Primary mechanisms of transport include the water supply and air dispersion. Many factors affect movements of chemicals throughout these media. However, a few chemical properties can provide a good screening-level indication of which pathway(s) a chemical is likely to take.

Water solubility is an indicator of the amount of chemical that will dissolve in aqueous solutions. Chemicals with high water solubility will readily dissolve. This indicates a potential for the chemical to be transported long distances in rain water and surface water runoff from the point of release. High water solubility also means the chemical is less likely to settle or precipitate as a solid at the bottom of a receiving stream; it may become dispersed throughout a drinking water supply that is eventually ingested by the general population. Water solubility is one of the criteria used in Section 4 to determine the potential for aquatic exposure and exposure to the general population via ingestion.

The octanol-water partition coefficient(Log K_{ow}) is a chemical-specific parameter that reflects the hydrophobicity of the chemical, meaning the tendency for the chemical to partition from water to organic phases (e.g. organic matter in soil or water, or lipids in organisms like fish). Some chemicals may initially be released on the ground; however, they are quickly absorbed by organic materials in the soil. In this instance, the chemical may never be transported to a water supply. Chemicals that readily dissolve in water are more likely to find their way to an underground water supply. The octanol-water partition coefficient is also used in Section 4 to evaluate aquatic exposure and general population exposure via ingestion. A high partition coefficient value means that the chemical is more soluble in octanol than in water while a low partition coefficient value means that the chemical is more soluble in water than in octanol.

Vapor pressure can be used to assess the amount of chemical that vaporizes into the gas phase (from solution or from a finished article). Similarly, the *Henry's Law Constant* indicates the amount of chemical that will volatilize from an aqueous solution. A high vapor pressure and Henry's Law Constant indicates a higher potential for the chemical to enter the vapor phase and be transported long distances through ambient air. These parameters are used in Section 4 to evaluate potential general population exposure via inhalation.

Persistence and Bioaccumulation

If a chemical is released, there still may be little or no potential for environmental and general population exposures. This potential is affected by the *fate* of the chemical in the environment and its ability for uptake by the receptor organism. Two parameters affecting fate components of the exposure pathway are persistence and bioaccumulation.

<u>Persistence</u>

Many natural phenomena can degrade or destroy chemicals. Factors that can contribute to degradation include exposure to light, reactivity with air and water and microbial activity. The ability of a chemical to persist in the environment can be measured by its half-life. This is the amount of time required for half of the chemical to be degraded. The half-life can be measured (or estimated) for different media (e.g., half-life in air and half-life in water). Chemicals with a very long half-life are said to be persistent. Half-life is used in Section 4 to describe the persistence of pentaBDE alternatives.

<u>Bioaccumulation</u>

The toxicological effects exhibited for some endpoints depend on the ability of the chemical to be absorbed in tissue, and remain for extended periods of time. This general concept is referred to as bioaccumulation. Chemicals that are highly bioaccumulative pose greater concerns. Bioaccumulation can be measured or estimated by analyzing a number of parameters, including the fish bioconcentration factor (BCF). BCFs are used in Section 4 to evaluate the bioaccumulation potential of each pentaBDE alternative.

3.3.2 Consumer Use and End-of-Life Analysis

Currently, there is uncertainty regarding the exposure pathways and routes associated with flame retardant chemicals such as pentaBDE. A significant amount of research is being conducted to assess their fate and transport from release points and consumer products to human and environmental receptors. The Furniture Flame Retardancy Partnership will evaluate the results of flame retardant exposure research as it is completed. This section very briefly discusses the potential pathways and routes of exposure associated with consumer uses and end-of-life (disposal) of flexible polyurethane foam.

Primary Consumer Uses (Furniture, Carpet Cushion and Mattresses)

In the United States today, pentaBDE is primarily used in flexible polyurethane foam for residential upholstered furniture and mattresses. A significant, secondary market for pentaBDE foam includes carpet cushion (rebond) manufacturing because large quantities of off-spec and recycled foam are used to manufacture this product. Millions of pounds of foam that is flame retarded with pentaBDE or an alternative have been, and will be, sold and used in homes throughout the United States as carpet cushions. Direct exposure to millions of consumers from these sources is possible.

<u>Inhalation Exposure</u>

As discussed earlier, inhalation exposure can occur from dust, vapor and mist. Flame retardant chemicals that are incorporated into polyurethane foam will not result in consumer exposure to mist. However, recent studies of indoor air quality suggest that volatilization of PBDEs from treated furniture foam results in human exposure to PBDEs via inhalation (Wilford et. Al., 2003; Harrad et.al., 2004). This poses a potential, long-term pathway for inhalation exposure. Reactive flame retardants may result in a lower potential for exposure than additive flame retardants because the flame retardant should be bound within the foam matrix and is expected to be less available for release and subsequent exposure.

<u>Dermal Exposure</u>

Dermal exposure is also possible from direct contact with furniture, carpet padding and mattresses that have been treated with flame retardant chemicals. This pathway and route for flame retardants in foam is difficult to assess or quantify because foam is typically covered by textiles or carpet. Still, there is potential for direct contact if the foam is exposed. Additionally, it is expected that as carpet padding ages, foam dust will be generated and become airborne with traffic on carpet. This presents a particular exposure potential for children, who spend time on the floor. Dermal exposure is also possible when volatile chemicals deposit onto dust that subsequently settles on household surfaces. This potential pathway is expected to be greater for additive chemicals than for reactives.

Ingestion

Ingestion is another route of exposure to consumers that should be considered during a risk evaluation. As for dermal exposure, young children can be similarly exposed to household dust containing flame retardants: children are known to ingest larger amounts of household dust than adults. Mouthing of furniture, bedding and other materials are also possible routes of exposure for young children.

Miscellaneous and Historical Consumer Uses (Automobiles)

PentaBDE and other flame retardants have been used in flexible and rigid foam seating and other components of automobile interiors. Industry has been shifting from pentaBDE in this application over the past several years. However, the foam in automobile seats must still meet appropriate fire safety standards. Therefore, flame retardants are still used. There is one additional pathway and route of exposure associated with foam in automobile seating that has not been previously discussed. Studies have shown that a phenomenon known as “fogging” occurs inside vehicles when components of plastics and foam volatilize during use and deposit on windshields, creating a film. This typically occurs due to the elevated temperatures in closed autos that are left in direct sunshine during summer months. Additive chemicals vaporize from foam at these high temperatures. Fogging is generally associated with plasticizers, but flame retardants and other additives can also volatilize and contribute to this effect (Akzo Nobel Central Research, 1996).

4.0 FLAME-RETARDANT ALTERNATIVES EVALUATIONS

In order to evaluate chemical alternatives for flame retarding furniture foam, all of the factors discussed in prior sections of this report must be considered, including toxicology, exposure, type of flame-retardant chemical, efficacy of use within existing manufacturing systems, availability and viability of non-chemical alternatives, cost and performance. As of the date of this report, performance testing was not available for the alternative flame-retardant chemicals.

This section summarizes the toxicological and exposure characteristics of each chemical in alternative flame-retardant formulations that are considered viable substitutes for pentaBDE use in flexible polyurethane foam. Chemical components less than 1 percent by weight were not considered in this assessment. The characteristics of the chemicals in each formulation are summarized qualitatively in Section 4.1 using a relative ranking scheme and more detailed characteristics of the chemicals in each formulation are presented in Section 4.2.

These evaluations of flame-retardants are not full risk assessments, but do provide screening-level information on the hazards and potential routes of exposure associated with the chemical components. Chemical risk is composed of two parts: toxicity (hazard) and exposure. Toxicity is the ability to cause harm to human health or in the environment. Exposure is the amount of material to which workers, the community or the environment come into contact. The toxicological information summarized in these evaluations is based on existing information and will provide the basis for identifying unmet data needs. The exposure potential is derived from simple criteria applied to the physical, chemical, and environmental fate properties of the chemicals. A full exposure assessment would consider the quantity, frequency, duration and route of exposure. Understanding the exposure routes and pathways is critical to conducting an exposure assessment. The concentration of a chemical in the mixture would factor into the overall exposure assessment and, therefore, the potential risk associated with the commercial formulations of the flame retardant alternatives.

4.1 Summary of Flame-Retardant Chemical Alternatives

Table 4-1 presents a qualitative summary of toxicological and exposure characteristics of the chemicals in each formulation considered in the alternatives analysis. The table qualitatively summarizes toxicological endpoints and exposure routes for each chemical, including seven human health effects, two ecotoxicity effects and two environmental endpoints and six routes of occupational, general population and aquatic exposure. Each of these endpoints is explained in Table 4-2.

Table 4-1 Toxicology and Exposure Summary

L = Low hazard concern
M = Moderate hazard concern
H = High hazard concern
N = No
Y = Yes
P = Yes for pure chemical
N/A = not available
*Ongoing studies may result in a change in this endpoint.
** Chemical concentrations are listed in descending order
L, M,* or *H = Endpoint assigned using estimated values and professional judgment (Structure Activity Relationships)

Company	Chemical	% in Formulation**	Human Health Effects: Cancer Hazard	Skin Sensitizer	Reproductive	Developmental	Neurological	Systemic	Mutagenicity	Ecotoxicity: Acute	Chronic	Environmental: Persistence	Bioaccumulation	Potential Routes of Exposure: Worker: Inhalation	Worker: Dermal	Worker: Ingestion	General Population: Inhalation	General Population: Dermal	General Population: Ingestion	Aquatic	Reactive or Additive?
Albemarle	ANTIBLAZE 180 and ANTIBLAZE 195																				
	Tris(1,3-dichloro-2-propyl)Phosphate CAS # 13674-87-8	95%	M	L	M	M	L	M	M	M	M	_L_	_L_	N	Y	Y	N	Y	Y	Y	Additive
Albemarle	ANTIBLAZE 182 and ANTIBLAZE 205																				
	Proprietary A Chloroalkyl phosphate (1)		M	L	M	M	L	M	M	M	M	_L_	_L_	N	Y	Y	N	Y	Y	Y	Additive
	Proprietary B Aryl phosphate		_L_	_L_	M*	M*	M	M*	_L_	H	_H_	_L_	_M_	N	Y	Y	N	Y	N	N	Additive
	Triphenyl Phosphate CAS # 115-86-6		_L_	L	L	L	L	M	L	H	M	_L_*	_L_	Y	Y	Y	Y	Y	Y	Y	Additive
Albemarle	ANTIBLAZE V500																				
	Proprietary C Chloroalkyl phosphate (2)		_M_	_M_	_M_*	_M_*	L	M	L	M	M	*	_L_	N	Y	Y	N	Y	Y	Y	Additive
	Proprietary B Aryl phosphate		_L_	_L_	M*	M*	M	M*	_L_	H	_H_	_L_	_M_	N	Y	Y	N	Y	N	N	Additive
	Triphenyl Phosphate CAS # 115-86-6		_L_	L	L	L	L	M	L	H	M	_L_*	_L_	Y	Y	Y	Y	Y	Y	Y	Additive
Albemarle	SAYTEX RX-8500																				
	Proprietary D Reactive brominated flame retardant		_L_	_M_			_M_	_M_	L	_M_	_M_	_L_	_L_	N	Y	Y	N	N	Y	Y	Reactive
	Proprietary B Aryl phosphate		_L_	_L_	M*	M*	M	M*	_L_	H	_H_	_L_	_M_	N	Y	Y	N	Y	N	N	Additive
	Triphenyl Phosphate CAS # 115-86-6		_L_	L	L	L	L	M	L	H	M	_L_*	_L_	Y	Y	Y	Y	Y	Y	Y	Additive
Albemarle	SAYTEX RZ-243																				
	Proprietary E Tetrabromophthalate diol diester		_L_		*	*		_M_*		_L_*		_L_	_L_	N	Y	Y	N	N	Y	Y	Additive
	Proprietary B Aryl phosphate		_L_	_L_	M*	M*	M	M*	_L_	H	_H_	_L_	_M_	N	Y	Y	N	Y	N	N	Additive
	Triphenyl Phosphate CAS # 115-86-6		_L_	L	L	L	L	M	L	H	M	_L_*	_L_	Y	Y	Y	Y	Y	Y	Y	Additive

Table 4-1 Toxicology and Exposure Summary

L = Low hazard concern
M = Moderate hazard concern
H = High hazard concern
L, M, or *H* = Endpoint assigned using estimated values and professional judgment (Structure Activity Relationships)

N = No
Y = Yes
P = Yes for pure chemical

N/A = not available
*Ongoing studies may result in a change in this endpoint.
** Chemical concentrations are listed in descending order

Company	Chemical	% in Formulation**	Human Health Effects							Ecotoxicity		Environmental		Potential Routes of Exposure							Reactive or Additive?
														Worker			General Population				
			Cancer Hazard	Skin Sensitizer	Reproductive	Developmental	Neurological	Systemic	Mutagenicity	Acute	Chronic	Persistence	Bioaccumulation	Inhalation	Dermal	Ingestion	Inhalation	Dermal	Ingestion	Aquatic	
Ameribrom	FR513																				
	Tribromoneopentyl Alcohol CAS # 36483-57-5		*M*	L	*M*	*M*	*M*	M	M	M*	*H*	L	*L*	Y	Y	Y	N	N	Y	Y	Reactive
Great Lakes	Firemaster 550																				
	Proprietary F Halogenated aryl ester		*L*		*M**	*M**		*M*		H	*L**	L	L	N	Y	Y	N	Y	N	N	Additive
	Proprietary G Triaryl phosphate, isopropylated		*L*	*L*	M*	M*	M	M	*L*	H	*H*	*L*	*M*	N	Y	Y	N	Y	N	N	Additive
	Triphenyl Phosphate CAS # 115-86-6		*L*	L	L	L	L	M	L	H	M	*L**	*L*	Y	Y	Y	Y	Y	Y	Y	Additive
	Proprietary H Halogenated aryl ester		*L*		*M**	*M**		*M*		H	*L**	L	L	N	Y	Y	N	Y	N	N	Additive
Great Lakes	Firemaster 552																				
	Proprietary F Halogenated aryl ester		*L*		*M**	*M**		*M*		H	*L**	L	L	N	Y	Y	N	Y	N	N	Additive
	Proprietary G Triaryl phosphate, isopropylated		*L*	*L*	M*	M*	M	M	*L*	H	*H*	*L*	*M*	N	Y	Y	N	Y	N	N	Additive
	Triphenyl Phosphate CAS # 115-86-6		*L*	L	L	L	L	M	L	H	M	*L**	*L*	Y	Y	Y	Y	Y	Y	Y	Additive
	Proprietary H Halogenated aryl ester		*L*		*M**	*M**		*M*		H	*L**	L	L	N	Y	Y	N	Y	N	N	Additive
Supresta	AB053																				
	Tris(1,3-dichloro-2-propyl)Phosphate CAS # 13674-87-8		M	L	M	M	L	M	M	M	M	*L*	*L*	N	Y	Y	N	Y	Y	Y	Additive
	Tris(2-chloroisopropyl) phosphate CAS # 13674-84-5		*M*	*M*	*M*	L	L	M	M	M	M	M	*L*	Y	Y	Y	Y	Y	Y	Y	Additive
Supresta	AC003																				
	Proprietary I Organic phosphate ester	92-99%	*L*	L	L	L	*L*	*M*	L	H	H	*H*	L	P	Y	Y	N	Y	Y	Y	Additive
	Triphenyl Phosphate CAS # 115-86-6	1-8%	*L*	L	L	L	L	M	L	H	M	*L**	*L*	Y	Y	Y	Y	Y	Y	Y	Additive

Table 4-1 Toxicology and Exposure Summary

L = Low hazard concern — N = No — N/A = not available
M = Moderate hazard concern — Y = Yes — *Ongoing studies may result in a change in this endpoint.
H = High hazard concern — P = Yes for pure chemical — ** Chemical concentrations are listed in descending order
L, M, or ***H*** = Endpoint assigned using estimated values and professional judgment (Structure Activity Relationships)

Company	Chemical	% in Formulation**	Human Health Effects							Ecotoxicity		Environmental		Potential Routes of Exposure							Reactive or Additive?
														Worker			General Population				
			Cancer Hazard	Skin Sensitizer	Reproductive	Developmental	Neurological	Systemic	Mutagenicity	Acute	Chronic	Persistence	Bioaccumulation	Inhalation	Dermal	Ingestion	Inhalation	Dermal	Ingestion	Aquatic	
Supresta	AC073																				
	Triphenyl Phosphate CAS # 115-86-6	38-48%	*L*	L	L	L	L	M	L	H	M	*L**	*L*	Y	Y	Y	Y	Y	Y	Y	Additive
	Proprietary J Aryl phosphate	40-46%	*L*	*L*	L		L	M	M*	*L*	*H*	*L*	*L*	Y	Y	Y	Y	Y	Y	Y	Additive
	Proprietary K Aryl phosphate	12-18%	*L*	*L*			*L*	*M*		*L*	*L*	*L*	*L*	P	Y	Y	N	Y	N	N	Additive
	Proprietary L Aryl phosphate	1-3%	*L*	*L*			*L*	*M*		*L*	*L*	*L*	*L*	P	Y	Y	N	Y	N	N	Additive
Supresta	Fyrol FR-2																				
	Tris(1,3-dichloro-2-propyl)phosphate CAS # 13674-87-8	70%	M	L	M	M	L	M	M	M	M	*L*	*L*	N	Y	Y	N	Y	Y	Y	Additive
	Tris(2-chloroisopropyl) phosphate CAS # 13674-84-5	20%	*M*	*M*	*M*	L	L	M	M	M	M	M	*L*	Y	Y	Y	Y	Y	Y	Y	Additive

Table 4-2 Definitions of Toxicological Endpoints

Toxicological Category	Toxicological Endpoint	Definition
Human Health Effects	Cancer Hazard	Chemical is known to induce malignancies.
	Skin Sensitizer	Skin reaction resulting from a single or multiple exposure characterized by the presence of inflammation; it may result in cell death.
	Reproductive	Produces non-heritable harmful effects on the progeny and/or an impairment of male and female reproductive function or capacity.
	Developmental*	Adverse effects on the developing organism (including structural abnormality, altered growth, or functional deficiency or death) resulting from exposure prior to conception (in either parent), during prenatal development, or postnatally up to the time of sexual maturation.
	Neurological	Adverse effects on the central or peripheral nervous system.
	Systemic*	Consequence that is of either a generalized nature or that occurs at a site distant from the point of entry of a substance: a systemic effect requires absorption and distribution of the substance in the body.
	Mutagenicity	Induction of heritable changes (mutations) in the genotype in a cell as a consequence of alterations or loss of genes or chromosomes (or parts thereof).
Ecotoxicity	Adverse effects observed in living organisms (fish, birds, plants, etc.) that typically inhabit the wild.	
	Acute	Short-term, in relation to exposure or effect. Exposures are typically less than 96 hours.
	Chronic	Effects observed after repeated exposures.
Environmental	Persistence	Attribute of a substance that describes the length of time that the substance remains in a particular environment before it is physically removed or chemically or biologically transformed. Physical removal typically involves shifting the substance from one medium to another (e.g, from air to water) but does not destroy the chemical of concern. Chemical and biological transformation result in permanent removal of the chemical from the environment which is preferable unless the chemical is transformed into hazardous byproducts.
	Bioaccumulation*	Ability of living organisms to concentrate a substance obtained either directly from the environment or indirectly through its food.

*REFERENCE: International Union of Pure and Applied Chemistry, Clinical Chemistry Division Commission on Toxicology. Glossary for Chemists of Terms Used in Toxicology (IUPAC Recommendations, 1993).

Each toxicological endpoint is assigned a rating of L, M, or H to indicate whether the chemical has a low (L), medium (M), or high (H) hazard. If the L, M, or H indicator is bold, then the assignment was made using experimental data on the chemical. If the L, M, or H indicator is hollow, then experimental data were not available for that chemical and the assignment was estimated using modeling techniques and professional judgment. Similarly, each exposure route is assigned a rating of Y (yes) or N (no) to indicate whether that exposure route is probable for each chemical.

4.1.1 Explanation of Toxicological Endpoints Rating

The assessments combine data on flame-retardant alternatives from four sources: (1) publicly available measured (experimental) data obtained from a comprehensive literature review; (2) measured confidential data from EPA OPPT Confidential Business Information (CBI) databases; (3) estimations from EPA's New Chemical Program's P2 Framework and Sustainable Futures predictive methods; and (4) professional judgment of EPA staff who identified experimental data on closely related analogs. When experimental data were lacking, the expert judgment of scientists from EPA's New Chemical Program was used to assess physical/chemical property, environmental fate, aquatic toxicity and human health endpoints. The following abbreviations are used to indicate sources of data presented in this assessment:

- M = Measured/experimental data contained in the open literature;
- MC = Measured/experimental confidential data contained in EPA OPPT CBI databases or submitted by industry;
- E = Estimations obtained using predictive methodology; and
- P = Professional judgment of subject matter experts.

Table 4-3 lists the criteria that were used to interpret the data collected in this document. These criteria are used by the EPA New Chemicals Program to assign concern levels to new chemicals submitted under the Toxic Substances Control Act (TSCA). EPA has published these criteria in several sources including USEPA 1992, USEPA 1994, and USEPA 1995. EPA New Chemicals Program persistence criteria have been published in the Federal Register (USEPA 1999).

More information on the EPA New Chemicals Program criteria used to assign concern levels can be found in the Sustainable Futures Pilot Project Interpretive Guidance Document (attached as Appendix B to this document) or visit:
http://www.epa.gov/oppt/newchems/sustainablefutures.htm.

Table 4-3 Criteria Used to Assign Concern Levels

Concern Level	**Persistence Criteria**
High	Half-life in water, soil, or sediment > 180 days
Moderate	Half-life in water, soil, or sediment between 60 and 180 days
Low	Half-life in water, soil, or sediment < 60 days
Concern Level	**Bioaccumulation Criteria**
High	Bioconcentration factor (BCF) > 5000
Moderate	BCF between 1,000 and 5,000
Low	BCF < 1,000
Concern Level *	**Aquatic Toxicity Criteria**
High	Value is < 1 mg/L (chronic value <0.1 mg/L)
Moderate	Value is between 1 and 100 mg/L (chronic value 0.1 and 10 mg/L)
Low	Value is >100 mg/L (chronic value >10 mg/L) or log K_{ow} is greater than 8

Concern Level	Human Health Criteria
High	Evidence of adverse effects in human populations *or* conclusive evidence of severe effects in animal studies
Moderate	Suggestive animal studies, analog data, *or* chemical class known to produce toxicity
Low	No concern identified

*If the water solubility is estimated, the chemical will not be considered to have "no effects at saturation" if the estimated value is within a factor of 10 percent of the cutoff value. The concern level will be considered low if "no effects at saturation" (below the solubility limit).

If measured data pertaining to these criteria are not available, they can be estimated based on several physical and chemical properties. Estimations for these properties were obtained using the models of EPA's P2 Framework. The P2 Framework is an approach to risk-screening that incorporates pollution prevention principles in the design and development of chemicals. These models are screening level methods and are intended to be used when data are unavailable or to supplement available data. They are not intended to replace data from well-designed studies. For physical/chemical properties and environmental fate parameters, estimates were obtained from the Estimations Program Interface for Windows (EPIWIN) suite methodology. These methods were used to obtain melting point, boiling point, vapor pressure, octanol/water partition coefficient, water solubility, Henry's Law constant, atmospheric oxidation rate, biodegradation potential, soil adsorption coefficient, bioconcentration factor, hydrolysis rate, volatilization rates and removal in a sewage treatment plant as applicable. For aquatic toxicity potential, EPA's Ecological Structure Activity Relationships (ECOSAR) estimation program was used. This methodology uses chemical structure to estimate toxicity of an industrial chemical to fish, invertebrates, and algae in the surface water to which the chemical has been discharged. The program determines both acute (short-term) toxicity and, when available, chronic (long-term or delayed) toxicity. The potential for a chemical to cause cancer in humans was estimated using OncoLogic. This program uses a decision-tree based on the known carcinogenicity of chemicals with similar chemical structures, information on mechanisms of action, short-term predictive tests, epidemiological studies, and expert judgment. All estimates obtained in this project were reviewed by EPA scientists with expertise in the appropriate field.

4.1.2 Explanation of Exposure Route Rating

Six exposure routes are presented for each chemical, including two occupational exposure routes, three general population exposure routes and one aquatic exposure route. Each of these potential routes is assigned a Y (yes, exposure may occur) or an N (no, exposure is not likely to occur). The assignment of a Y or an N is determined from specific criteria related to the physicochemical characteristics of the chemical as it exists in the formulated product. The assignment of a P indicates where worker exposure may result from the pure chemical.
The exposure routes are based on the state of the pure compound or representative pure compound unless further use information has been provided. The thresholds for each exposure route were adopted from EPA's New Chemicals Program, except as noted.

Occupational Exposure

Inhalation

Liquids[1]: If a liquid has a vapor pressure amenable to volatilization, then the liquid will evaporate and present the potential for a person to inhale the vapor. Occupational exposure may occur when the vapor pressure is greater than 1 x 10^{-06} mm Hg at 25 degrees Celsius. Liquids may also be inhaled as a mist if the liquid chemical is sprayed during transfer or application operations.

Solids[2]: Occupational exposure may occur in all cases when processing or handling solids. Solid-state chemicals may be used in a crystalline, packed, or powder form. In all cases, a solid chemical may produce particulate dust as a byproduct of manufacturing or use operations. When this occurs, a worker may inhale the dust particles while working with the chemical.

Gases[3]: Occupational exposure may occur in all cases when processing or handling gases. Gaseous chemicals should always be contained in cylinders to enable their use; however, if they are uncontained, gaseous chemicals result in exposure to workers. Routine exposure to gaseous chemicals is not expected unless there is an accident. However, fugitive releases may occur when connecting transfer lines.

Dermal

Dermal exposures may occur to workers while handling liquid or solid flame-retardant chemicals. In general, workers handling liquid chemicals may be exposed to the chemical by full hand immersion, splashing, or spraying depending upon the manufacturing processes utilized at a facility. Workers handling solid chemicals can be exposed on the surface of their hands as well as from particulate dust that may settle onto their skin. All chemicals are expected to present a dermal exposure to workers in this report. The use of personal protective equipment may mitigate these exposures.

Ingestion

Exposures associated with ingestion are not included for the purposes of this screening level assessment; however, workers may incidentally ingest flame-retardant chemicals through ingestion of contaminated food and water. Ingestion may occur if the chemical is suspended in air as a particulate or a mist as part of manufacturing, and then recondenses or flocculates into food or drinking sources. Alternatively, secondary ingestion may occur as a result of inhaling the mist or dust form of the chemical, and then swallowing residual chemical in the nasal or esophageal passageways.

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[1] Liquids are substances that have a melting point less than 25 degrees Celsius and a boiling point greater than 25 degrees Celsius.
[2] Solids are substances that have a melting point of greater than 25 degrees Celsius.
[3] Gases are substances that have a boiling point less than 25 degrees Celsius.

General Population Exposure

Inhalation

Liquids[4]: If the liquid has a vapor pressure amenable to volatilization from the product in which the chemical is carried, a person may inhale the liquid as a vapor while in contact with the product or substance carrying the chemical. For this report, general population exposure may occur if the chemical vapor pressure is greater than 1×10^{-06} mm Hg at 25 degrees Celsius and if the chemical is additive, not reactive[5].

Solids[6]: General population exposure may occur if the vapor pressure is greater than 1×10^{-06} mm Hg at 25 degrees Celsius and if the chemical is not reactive. Although not included in this screening level assessment, as foam products age and break down, particulate (matter) may be released from the foam products which may contain flame-retardant chemicals. This flame-retardant foam dust may be present in carpets or in flame-retardant furniture and could represent an exposure to the general population.

Gases[7]: General population exposure is not expected to occur if the chemical is a gas, since gases would not be intentionally contained outside of the manufacturing arena (excluding accidental releases).

Dermal

Dermal exposures may occur to the general population while handling products or substances containing the flame-retardant chemical, if the flame-retardant chemical is not reactive.

Ingestion

The general population may be exposed to a flame-retardant chemical if the chemical has water solubility greater than 1×10^{-06} grams/liter, is dispersible, or has the potential to leach. These would indicate that the chemical is easily absorbed in water and may be found in surface and groundwater sources as a result of disposal and environmental releases of the chemical.

Aquatic Exposure

The flame-retardant chemical may present an aquatic exposure if the water solubility of the compound is greater than 1×10^{-06} grams/liter or the compound is dispersible in water.

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[4] Liquids are substances that have a melting point less than 25 degrees Celsius and a boiling point greater than 25 degrees Celsius.

[5] Reactive chemicals (as opposed to additive chemicals) are those that are incorporated into the foam by new chemical bonds that are formed between the substrate and the flame retardant. Therefore, they are not assumed to be available for exposure.

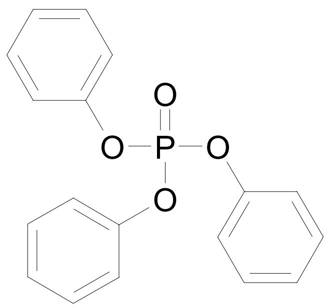
[6] Solids are substances that have a melting point of greater than 25 degrees Celsius.

[7] Gases are substances that have a boiling point less than 25 degrees Celsius.

4.2 Chemical Summary Assessments

The following subsections (4.2.1 through 4.2.19) contain summaries of the toxicity and exposure data for 19 chemicals that are components of the flame retardant formulations assessed in this report. These summary data were used to develop the hazard and exposure conclusions that are presented in Table 4-1. The studies from which these data were derived are summarized in Volume 2 of this report, entitled Chemical Hazard Reviews.

4.2.1 Triphenyl Phosphate

Record ID: Triphenyl Phosphate	**CAS No.** 115-86-6
	**MW**: 326.29
	MF: $C_{18}H_{15}O_4P$
	Physical Forms: **Neat:** Solid **As Formulated:**
	Use: Flame retardant, additive
SMILES: c1ccccc1OP(=O)(Oc2ccccc2)Oc3ccccc3	
Name: Phosphoric acid, triphenyl ester	
Synonyms: Triphenyl phosphate; TPP	

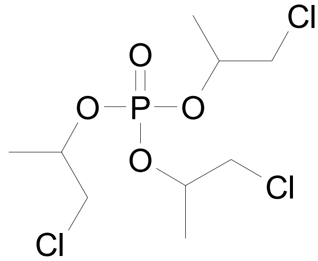
ASSESSMENT SUMMARY:			
Concern Level	**HIGH**	**MODERATE**	**LOW**
Persistence			**X**
Bioconcentration			**X**
Cancer Health Hazard			**X**
Non-Cancer Health Hazard		**X**	
Aquatic Toxicity Hazard	**X**		
Is the chemical predicted to be a PBT by PBT Profiler?	**No**		
Overall Hazard Concern	**Human Health Hazard: Moderate** **Aquatic Hazard: High**		

Record ID: Triphenyl Phosphate		**CAS No.** 115-86-6
PHYSICAL/CHEMICAL PROPERTIES		
Melting Point (deg C)	50.5 (M)	
Boiling Point (deg C)	245 @ 11 mm Hg (M); 389 (E)	
Vapor Pressure (mm Hg)	6.3×10^{-6} (M)	
Water Solubility (g/L)	1.9×10^{-3} (M)	
Log K_{ow}	4.59 (M)	
ENVIRONMENTAL TRANSPORT AND FATE:		
Transport		
Henry's Law Constant – HLC (atm-m^3/mole)	3.98×10^{-8} (E)	
Soil Adsorption Coefficient – K_{oc}	5200 (E)	
Bioconcentration Factor – BCF	113 (E)	
Persistence		
Experimental Biodeg Tests		
Ultimate Biodeg Model	Weeks-months (E)	
Primary Biodeg Model	Days (E)	
BOD or COD		
Atmospheric Half-life	12 hours (E)	
Hydrolysis Half-life		
Volatilization Half-life for Model River	13 days (E)	
Volatilization Half-life for Model Lake	152 days (E)	
Removal in Sewage Treatment Plant	61% (E)	
Ready Biodegradability	Not ready biodegradable (E)	
Byproducts		
Degradation Products		
Metabolites		
ECOTOXICITY:		
ECOSAR Class	Esters-phosphate	
Comments	*** = based on geometric mean of experimental values**	

Record ID: Triphenyl Phosphate	**CAS No.** 115-86-6
Acute Toxicity	
Fish LC_{50}	96-h LC50, 0.870 mg/L (M)
Daphnid LC_{50}	48-h LC50, 1.2 mg/L (MC) 48-h LC50, 1.1 mg/L* (M)
Green Algae EC_{50}	96-h EC50, 2.0 mg/L (M)
Chronic Toxicity	
Fish ChV	0.140 mg/L (MC)
Daphnid ChV	0.1 mg/L (D48/ACR10) (MC, M)
Green Algae ChV	≥0.140 mg/L (E) < 0.600 mg/L (M) 0.5 mg/L (A96/ACR4) (M)
Overall Hazard Concern for Aquatic Toxicity	HIGH
HEALTH EFFECTS:	
Absorption	Poor thru skin as neat solid, moderate thru skin in solution; moderate thru lungs and GI tract based on closely related analogs (P)
CANCER HEALTH EFFECTS:	
Experimental data	
OncoLogic Results	Marginal (E)
Overall Hazard Concern for Carcinogenicity	LOW
NON-CANCER HEALTH EFFECTS:	
Acute Toxicity	Low; Rat, mouse, rabbit, oral, LD50 > 5000 mg/kg (M); Mammal, dermal, LD50 > 8000 mg/kg (MC); rabbit, dermal, LD50 > 7900 mg/kg (M)
Eye Irritation	Moderate; Mild eye irritation, rabbits (M, MC)
Skin Irritation	Low; Negative, rabbits (M)
Skin Sensitizer	Low; negative in guinea pigs (MC), very low incidence in humans (M)
Reproductive Effects	Low; 91-112-d reproductive (incomplete)/developmental study, rats, diet, no reproductive effects, NOAEL = 690 mg/kg/day (1%) (M)

Record ID: Triphenyl Phosphate	CAS No. 115-86-6
Developmental Effects	Low; 91-112-d reproductive/developmental study, rats, diet, no developmental effects, NOAEL = 690 mg/kg/day, maternal LOAEL = 690 mg/kg/day (1%) (M)
Immune System Effects	Low; 120-d repeated-dose study, rats, diet, no immune system effects, NOAEL = 700 mg/kg/day (1%) (M)
Neurotoxicity	Low; negative in delayed neurotoxicity studies in the hen at up to 10,000 mg/kg/day (oral, 6 dosing days) and in the cat at 700 mg/kg (subcutaneous, single dose) (M); 120-d repeated-dose neurotoxicity screening study, rats, diet, no neurobehavioral effects, NOAEL = 711 mg/kg/day (1.0%) (M)
Genotoxicity/Mutagenicity	Low; Negative in Ames assay and Negative in forward mutation assay, mouse lymphoma cells *in vitro*, with and without metabolic activation (M); Negative in mitotic gene conversion assay in *Saccharomyces cerevisiae* with and without activation (M)
Systemic Effects	Moderate; 35-d repeated-dose study (inadequate), rats, diet, increased relative liver weight at 0.5%, NOAEL = 0.1%; 120-d repeated-dose (neurotoxicity screening) study, rats, diet, decreased body weight gain without decreased food consumption, NOAEL = 161 mg/kg/day (0.25%), LOAEL = 345 mg/kg/day (1%); 21-d repeated-dose study (inadequate), rabbits, dermal, systemic effects (M)
Overall Hazard Concern for Non-Cancer Health Effects	MODERATE

4.2.2 Tris(2-Chloroisopropyl) Phosphate

Record ID: Tris (2-chloroisopropyl) phosphate	**CAS No.** 13674-84-5
	**MW**: 327.57
	MF: $C_9H_{18}Cl_3O_4P$
	Physical Forms: **Neat:** Liquid **As Formulated:**
	Use: Flame retardant, additive
SMILES: ClCC(C)OP(=O)(OC(C)CCl)OC(C)CCl	
Name: 2-Propanol, 1-chloro-, phosphate (3:1)	
Synonyms: Tris (2-chloroisopropyl) phosphate; TCPP	

ASSESSMENT SUMMARY:

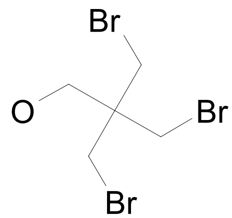
Concern Level	HIGH	MODERATE	LOW
Persistence		X	
Bioconcentration			X
Cancer Health Hazard		X	
Non-Cancer Health Hazard		X	
Aquatic Toxicity Hazard		X	
Is the chemical predicted to be a PBT by PBT Profiler?	**No**		
Overall Hazard Concern	**Human Health Hazard: Moderate** **Aquatic Hazard: Moderate**		

Record ID: Tris (2-chloroisopropyl) phosphate	CAS No. 13674-84-5
PHYSICAL/CHEMICAL PROPERTIES	
Melting Point (deg C)	-40 (M)
Boiling Point (deg C)	Decomposes at 244 (M)
Boiling Point Pressure (mm Hg)	
Vapor Pressure (mm Hg)	$5.64x10^{-5}$ (M)
Water Solubility (g/L)	1.2 (M)
Log K_{ow}	2.59 (M)
ENVIRONMENTAL TRANSPORT AND FATE:	
Transport	
Henry's Law Constant – HLC	$5.96x10^{-8}$ atm-m^3/mole (E)
Soil Adsorption Coefficient – K_{oc}	1278 (E)
Bioconcentration Factor – BCF	3.3 (E)
Persistence	
Experimental Biodeg Tests	14% Biodegradation in 28 days (M) 21% Biodegradation in 28 days by O2 uptake (M) 0% Biodegradation in 28 days with activated sludge by BOD (M)
Ultimate Biodeg Model	Months (E)
Primary Biodeg Model	Days-Weeks (E)
BOD or COD	
Atmospheric Half-life	2.9 hours (E)
Hydrolysis Half-life	
Volatilization Half-life for Model River	Negligible (E)
Volatilization Half-life for Model Lake	Negligible (E)
Removal in Sewage Treatment Plant	3.38% (E)
Ready Biodegradability	Not ready biodegradable (M)
Byproducts	
Degradation Products	

Record ID: Tris (2-chloroisopropyl) phosphate	**CAS No.** 13674-84-5
Metabolites	
ECOTOXICITY:	
ECOSAR Class	Ester-phosphate
Comments	* = based on geometric mean of NOEC and LOEC
Acute Toxicity	
Fish LC_{50}	96-h LC50, 51 mg/L (M)
Daphnid LC_{50}	48-h LC50, 131 mg/L (M)
Green Algae EC_{50}	96-h EC50, 47.0 mg/L (M)
Chronic Toxicity	
Fish ChV	5.1 mg/L (F96/ACR10) (M)
Daphnid ChV	13.0 mg/L (D48/ACR10) (M)
Green Algae ChV	10.0 mg/L (M)
Overall Hazard Concern for Aquatic Toxicity	MODERATE
HEALTH EFFECTS:	
Absorption	Good absorption and reaction, all routes (P)
CANCER HEALTH EFFECTS:	
Experimental data	Moderate by analogy to a closely related compound, 2-yr carcinogenicity study, rats, renal tubule adenomas (P)
OncoLogic Results	Moderate (E)
Overall Hazard Concern for Carcinogenicity	MODERATE

Record ID: Tris (2-chloroisopropyl) phosphate	**CAS No.** 13674-84-5
NON-CANCER HEALTH EFFECTS:	
Acute Toxicity	Low; Rat oral LD_{50} = 1546-3800 mg/kg (male), 1017-3400 mg/kg (female); Rat 4-h inhalation LC_{50} > 4.6 mg/L; >5 mg/L (males), ~5.0 mg/L (females); Rabbit dermal LD_{50} > 2000 mg/kg (M)
Eye Irritation	Moderate; Slight eye irritant (M)
Skin Irritation	Moderate; Slight skin irritant (M)
Skin Sensitizer	Moderate; Uncertain concern for sensitization because substance is potentially an alkylating agent (P)
Reproductive Effects	Moderate by analogy to a closely related compound; reproductive study, mice, oral, 175, 350, 700 mg/kg/day, sperm endpoints affected, decreased fertility and litter size, LOAEL = 175 mg/kg/day (P)
Developmental Effects	Low; Developmental toxicity study, rats, diet, NOAEL = 625 mg/kg (M)
Immune System Effects	
Neurotoxicity	Low; No evidence of delayed neurotoxicity in hens (M)
Genotoxicity/Mutagenicity	Moderate; Negative, mutagenicity, *Salmonella* (M); Positive, mutagenicity, mouse lymphoma, with activation (M); Weakly positive, unscheduled DNA synthesis (UDS) (MC); Negative, cell transform (MC); Negative, chromosomal aberration, rat, *in vivo* (MC)
Systemic Effects	Moderate; 90-d repeated-dose study, rats, diet, effects on liver, kidney, bone marrow, thyroid, NOAEL = 800 ppm (males), 7500 ppm (females) (M, P)
Overall Hazard Concern for Non-Cancer Health Effects	MODERATE

4.2.3 Tribromoneopentyl alcohol

Record ID: Tribromoneopentyl alcohol	**CAS No.** 36483-57-5
	**MW**: 324.84 **MF:** $C_5H_9Br_3O$ **Physical Forms:** **Neat:** Solid **As Formulated:** **Use:** Flame retardant, reactive
SMILES: OCC(CBr)(CBr)CBr	
Name: 1-Propanol, 2,2-dimethyl-, tribromo derivative	
Synonyms: Tribromoneopentyl alcohol, TBNPA	

ASSESSMENT SUMMARY:

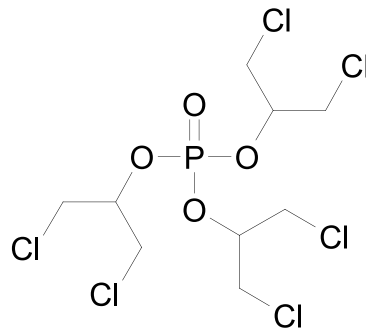
Concern Level	**HIGH**	**MODERATE**	**LOW**
Persistence			**X**
Bioconcentration			**X**
Cancer Health Hazard		**X**	
Non-Cancer Health Hazard		**X**	
Aquatic Toxicity Hazard	**X**		
Is the chemical predicted to be a PBT by PBT Profiler?	**No**		
Overall Hazard Concern	**Human Health Hazard: Moderate** **Aquatic Hazard: High**		

Record ID: Tribromoneopentyl alcohol		CAS No. 36483-57-5
PHYSICAL/CHEMICAL PROPERTIES		
Melting Point (deg C)	62-67 (M)	
Boiling Point (deg C)	300 (E)	
Boiling Point Pressure (mm Hg)	760 (E)	
Vapor Pressure (mm Hg)	6.2×10^{-5} (E)	
Water Solubility (g/L)	2 (M)	
Log K_{ow}	2.25 (E)	
ENVIRONMENTAL TRANSPORT AND FATE:		
Transport		
Henry's Law Constant – HLC	1.14×10^{-10} atm-m^3/mole (E)	
Soil Adsorption Coefficient – K_{oc}	22.9 (E)	
Bioconcentration Factor – BCF	10.8 (E)	
Persistence		
Experimental Biodeg Tests	2.5% CO2 evolution over 28 days in OECD 310 test (MC); 77% removal as DOC using OECD 302B in 36 days after a 10-day lag period (MC)	
Ultimate Biodeg Model	Weeks-months (E)	
Primary Biodeg Model	Days-weeks (E)	
BOD or COD		
Atmospheric Half-life	25 hours (E)	
Hydrolysis Half-life		
Volatilization Half-life for Model River	Negligible (E)	
Volatilization Half-life for Model Lake	Negligible (E)	
Removal in Sewage Treatment Plant	2.55% (E)	
Ready Biodegradability	Not ready biodegradable (MC)	
Byproducts		
Degradation Products		
Metabolites		

Record ID: Tribromoneopentyl alcohol	**CAS No.** 36483-57-5
ECOTOXICITY:	
ECOSAR Class	Haloalcohols
Acute Toxicity	
Fish LC_{50}	96-h LC50, < 11.0 mg/L (E)
Daphnid LC_{50}	48-h LC50, < 11.0 mg/L (E)
Green Algae EC_{50}	96-h EC50, ≤ 0.240 mg/L (E)
Chronic Toxicity	
Fish ChV	< 1.2 mg/L (E)
Daphnid ChV	< 2.0 mg/L (E)
Green Algae ChV	≤ 0.030 mg/L (E)
Overall Hazard Concern for Aquatic Toxicity	HIGH
HEALTH EFFECTS:	
Absorption	Nil thru skin as neat material; moderate thru skin when in solution; good absorption expected thru lungs and GI tract (P)
CANCER HEALTH EFFECTS:	
Experimental data	Moderate by analogy to a closely related compound; 2-yr study, male/female, rats, mice, neoplasms in multiple organs (P)
OncoLogic Results	Moderate
Overall Hazard Concern for Carcinogenicity	MODERATE

Record ID: Tribromoneopentyl alcohol		CAS No. 36483-57-5
NON-CANCER HEALTH EFFECTS:		
Acute Toxicity	Low; Rat oral LD_{50} = 1630 mg/kg, effects on bladder; Rat dermal LD_{50} >2000 mg/kg; Rat 7-h inhalation LC_{50} > 714 mg/m^3 (mixture, inadequate study) (M)	
Eye Irritation	Moderate; Mild eye irritant in rabbits (M)	
Skin Irritation	Moderate; Mild skin irritant in rabbits 24 hr exposure (M) but not 4 hour exposure (MC)	
Skin Sensitizer	Low; negative in mouse local lymph node assay (MC)	
Reproductive Effects	Moderate by analogy to a closely related compound; repro/fertility study, mice, diet, 141, 274, 589 mg/kg/day, decreased fertility and litter size, increased gestation length, LOAEL = 141 mg/kg/day (P)	
Developmental Effects	Moderate by analogy to a closely related compound; repro/fertility study, mice, diet, 141, 274, 589 mg/kg/day, decreased pup weight, NOAEL = 141 mg/kg/day (P)	
Immune System Effects		
Neurotoxicity	Moderate based on bromo substituents (P)	
Genotoxicity/Mutagenicity	Moderate; Positive, chromosomal aberrations, *in vitro* (MC); Positive, mouse micronucleus assay, females (MC); Positive, *Salmonella* with activation from hamster S9 (M); Negative, *Salmonella* without activation or with activation by rat S9 (M); Negative, yeast, mitotic gene conversion assay with or without activation (M)	
Systemic Effects	Moderate; 30-d repeated-dose study, rats, oral, diet, 10, 30, 100, 300 mg/kg/day, kidney, ureter, bladder, blood changes, NOAEL = 30 mg/kg/day (M,P)	
Overall Hazard Concern for Non-Cancer Health Effects	MODERATE	

4.2.4 Tris(1,3-dichloro-2-propyl) Phosphate

Record ID: Tris(1,3-dichloro-2-propyl) Phosphate	**CAS No.** 13674-87-8
	**MW**: 430.91
	MF: $C_9H_{15}Cl_6O_4P$
	Physical Forms: **Neat:** Liquid **As Formulated:**
	Use: Flame retardant, additive

SMILES: ClCC(CCl)OP(=O)(OC(CCl)CCl)OC(CCl)CCl
Name: 2-Propanol, 1,3-dichloro-, phosphate (3:1)
Synonyms: Tris(1,3-dichloro-2-propyl) Phosphate, TDCPP; TDCP
ASSESSMENT SUMMARY:

Concern Level	HIGH	MODERATE	LOW
Persistence			X
Bioconcentration			X
Cancer Health Hazard		X	
Non-Cancer Health Hazard		X	
Aquatic Toxicity Hazard		X	
Is the chemical predicted to be a PBT by PBT Profiler?	**No**		
Overall Hazard Concern	**Human Health Hazard: Moderate** **Aquatic Hazard: Moderate**		

Record ID: Tris(1,3-dichloro-2-propyl) Phosphate	**CAS No.** 13674-87-8
PHYSICAL/CHEMICAL PROPERTIES	
Melting Point (deg C)	-58 (M)
Boiling Point (deg C)	236-237 @ 5 mm Hg (M); Slowly decomposes >200 (M)
Vapor Pressure (mm Hg)	$<10^{-6}$ (M)
Water Solubility (g/L)	0.042 (M)
Log K_{ow}	2.40 (M)
ENVIRONMENTAL TRANSPORT AND FATE:	
Transport	
Henry's Law Constant – HLC (atm-m^3/mol)	2.61×10^{-9} (E)
Soil Adsorption Coefficient – K_{oc}	9222 (E)
Bioconcentration Factor – BCF	2.3 (E)
Persistence	
Experimental Biodeg Tests	
Ultimate Biodeg Model	Recalcitrant (E)
Primary Biodeg Model	Weeks (E)
BOD or COD	
Atmospheric Half-life	7.1 hours (E)
Hydrolysis Half-life	
Volatilization Half-life for Model River	Negligible (E)
Volatilization Half-life for Model Lake	Negligible (E)
Removal in Sewage Treatment Plant	3 (E)
Ready Biodegradability	Not ready biodegradable (E)
Byproducts	
Degradation Products	
Metabolites	

Record ID: Tris(1,3-dichloro-2-propyl) Phosphate	CAS No. 13674-87-8
ECOTOXICITY:	
ECOSAR Class	Esters - phosphate
Comments	* = based on geometric mean of experimental values
Acute Toxicity	
Fish LC_{50}	96-h LC50, 1.9 mg/L* (M,MC)
Daphnid LC_{50}	48-h LC50, 3.8 mg/L (M)
Green Algae EC_{50}	96-h EC50, 12.0 mg/L (M)
Chronic Toxicity	
Fish ChV	0.200 mg/L* (F96/ACR10) (M, MC)
Daphnid ChV	0.400 mg/L (D48/ACR10) (M)
Green Algae ChV	6.0 mg/L (M)
Overall Hazard Concern for Aquatic Toxicity	MODERATE
HEALTH EFFECTS:	
Absorption	Good absorption and reaction, all routes
CANCER HEALTH EFFECTS:	
Experimental data	2-yr chronic toxicity/carcinogenicity study, rats, diet, 5, 20, 80 mg/kg/day, increased benign adrenal cortex tumors, testicular interstitial cell tumors, and hepatocellular adenomas at 20 and 80 mg/kg/day (M)
OncoLogic Results	Moderate
Overall Hazard Concern for Carcinogenicity	MODERATE
NON-CANCER HEALTH EFFECTS:	
Acute Toxicity	Low; Mouse oral LD_{50}= (male) 2670 & (female) 2250 mg/kg; Rat oral LD_{50} = 3160 mg/kg; Rabbit oral LD_{50} = 6800 mg/kg; Rabbit dermal (24-hr) LD_{50} >4640 mg/kg (no death, clinical signs or gross necropsy lesions)(M)
Eye Irritation	Moderate; Mild reversible conjunctival irritant or negative, rabbits (M)
Skin Irritation	Moderate; 4 Hrs: non-irritant; 24 hrs: mild skin irritant, rabbits (M)
Skin Sensitizer	Low; Negative in guinea pigs (MC); Uncertain concern for sensitization as substance is a potential alkylating agent (P)

Record ID: Tris(1,3-dichloro-2-propyl) Phosphate	CAS No. 13674-87-8
Reproductive Effects	Moderate; Male reproduction study, rabbits, gavage, 12-wk exposure, no effects on male fertility or spermatogenesis, NOAEL = 200 mg/kg/day (M); 2-yr chronic toxicity/carcinogenicity study, rats, diet, 5, 20, 80 mg/kg/day, anomalies of the testes and seminal vesicles, NOAEL = 5 mg/kg/day (M)
Developmental Effects	Moderate; Developmental toxicity study, gavage, rats, gd 6-15, 25, 100, 400 mg/kg/day, increased resorptions, decreased fetal viability, weight, and length, NOAEL = 100 mg/kg/day. Developmental toxicity study, gavage, rats, gd 7-19, 25, 50, 100, 200, 400 mg/kg/day, decreased fetal viability, NOAEL = 200 mg/kg/kday (M).
Immune System Effects	Low; Uncertain concern for immunotoxicity because substance is potentially an alkylating agent; Immunotoxicity assay, subcutaneous, mouse, 4 consecutive days, 0.25, 2.5, 25 mg/kg/day; lymphoid depletion of thymus, reduced responses to T-cell & B-cell antigens, NOAEL 0.25 mg/kg/day (M)
Neurotoxicity	Low; Acute delayed neurotoxicity study, hens, gavage, , no significant inhibition of brain neurotoxic esterase (NTE) activity at 10,000 mg/kg; 90-d study, hens, gavage, no behavioral effects or histopathological changes indicative of neurotoxicity, NOAEL = 100 mg/kg/day; In developmental toxicity assay, rats, gavage gd 7-19, no adverse effect on postnatal neurobehavioral tests of sensory and motor function, NOAEL = 200 mg/kg/day (M)
Genotoxicity/ Mutagenicity	Moderate; Positive, mutagenicity, *Salmonella*, with metabolic activation; Negative, mutagenicity, mouse lymphoma cells with or without activation & hamster lung cells with activation, *in vitro*; Negative, sex-linked recessive lethal, *Drosophila in vivo* (M) Positive only with activation, chromosomal aberrations, *in vitro*, human lymphocytes (MC) & mouse lymphoma cells (M); Negative, chromosomal aberrations, *in vitro,* Chinese hamster ovary cells (MC); Negative, sister chromatid exchange, *in vitro*, cell line not reported (MC); Positive with or without activation, sister chromatid exchange, *in vitro,* mouse lymphoma cell; Negative, chromosomal aberrations, *in vivo*, mice (M)
Systemic Effects	Moderate; 2-yr chronic toxicity/carcinogenicity study, rats, diet, 5, 20, 80 mg/kg/day, increased mortality, decreased body weight, anemia, anomalies of the liver, kidneys, testes, seminal vesicles, renal cortex, and adrenal cortex, LOAEL = 5 mg/kg/day. Inadequate 90-day dietary study, mice, 0.01, 0.04, 0.13, 0.42 and 1.33% in diet; increased mortality, decreased body weight, anemia, increased liver & kidney weight, liver histopathology; NOAEL= 0.01% dietary level (M)

Record ID: Tris(1,3-dichloro-2-propyl) Phosphate		**CAS No.** 13674-87-8
Overall Hazard Concern for Non-Cancer Health Effects	MODERATE	

4.2.5 Proprietary A

Record ID: Proprietary A: Chloroalkyl phosphate (1)			**CAS No.**
			MW:
			MF:
			Physical Forms: **Neat:** Liquid **As Formulated:**
			Use: Flame retardant, additive
SMILES:			
Name: Chloroalkyl phosphate (1)			
Synonyms:			
ASSESSMENT SUMMARY:			
Concern Level	**HIGH**	**MODERATE**	**LOW**
Persistence			**X**
Bioconcentration			**X**
Cancer Health Hazard		**X**	
Non-Cancer Health Hazard		**X**	
Aquatic Toxicity Hazard		**X**	
Is the chemical predicted to be a PBT by PBT Profiler?	**No**		
Overall Hazard Concern	**Human Health Hazard: Moderate** **Aquatic Hazard: Moderate**		

Record ID: Proprietary A: Chloroalkyl phosphate (1)	CAS No.
PHYSICAL/CHEMICAL PROPERTIES	
Melting Point (deg C)	-58 (M)
Boiling Point (deg C)	236-237 @ 5 mm Hg (M); Slowly decomposes >200 (M)
Vapor Pressure (mm Hg)	$<10^{-6}$ (M)
Water Solubility (g/L)	0.042 (M)
Log K_{ow}	2.40 (M)
ENVIRONMENTAL TRANSPORT AND FATE:	
Transport	
Henry's Law Constant – HLC (atm-m^3/mol)	2.61×10^{-9} (E)
Soil Adsorption Coefficient – K_{oc}	9222 (E)
Bioconcentration Factor – BCF	2.3 (E)
Persistence	
Experimental Biodeg Tests	
Ultimate Biodeg Model	Recalcitrant (E)
Primary Biodeg Model	Weeks (E)
BOD or COD	
Atmospheric Half-life	7.1 hours (E)
Hydrolysis Half-life	
Volatilization Half-life for Model River	Negligible (E)
Volatilization Half-life for Model Lake	Negligible (E)
Removal in Sewage Treatment Plant	3 (E)
Ready Biodegradability	Not ready biodegradable (E)
Byproducts	
Degradation Products	
Metabolites	

Record ID: Proprietary A: Chloroalkyl phosphate (1)	CAS No.
ECOTOXICITY:	
ECOSAR Class	Esters - phosphate
Comments	* = based on geometric mean of experimental values
Acute Toxicity	
Fish LC_{50}	96-h LC50, 1.9 mg/L* (M,MC)
Daphnid LC_{50}	48-h LC50, 3.8 mg/L (M)
Green Algae EC_{50}	96-h EC50, 12.0 mg/L (M)
Chronic Toxicity	
Fish ChV	0.200 mg/L* (F96/ACR10) (M, MC)
Daphnid ChV	0.400 mg/L (D48/ACR10) (M)
Green Algae ChV	6.0 mg/L (M)
Overall Hazard Concern for Aquatic Toxicity	MODERATE
HEALTH EFFECTS:	
Absorption	Good absorption and reaction, all routes
CANCER HEALTH EFFECTS:	
Experimental data	2-yr chronic toxicity/carcinogenicity study, rats, diet, 5, 20, 80 mg/kg/day, increased benign adrenal cortex tumors, testicular interstitial cell tumors, and hepatocellular adenomas at 20 and 80 mg/kg/day (M)
OncoLogic Results	Moderate
Overall Hazard Concern for Carcinogenicity	MODERATE
NON-CANCER HEALTH EFFECTS:	
Acute Toxicity	Low; Mouse oral LD_{50}= (male) 2670 & (female) 2250 mg/kg; Rat oral LD_{50} = 3160 mg/kg; Rabbit oral LD_{50} = 6800 mg/kg; Rabbit dermal (24-hr) LD_{50} >4640 mg/kg (no death, clinical signs or gross necropsy lesions)(M)
Eye Irritation	Moderate; Mild reversible conjunctival irritant or negative, rabbits (M)
Skin Irritation	Moderate; 4 Hrs: non-irritant; 24 hrs: mild skin irritant, rabbits (M)
Skin Sensitizer	Low; Negative in guinea pigs (MC); Uncertain concern for sensitization as substance is a potential alkylating agent (P)

Record ID: Proprietary A: Chloroalkyl phosphate (1)	CAS No.
Reproductive Effects	Moderate; Male reproduction study, rabbits, gavage, 12-wk exposure, no effects on male fertility or spermatogenesis, NOAEL = 200 mg/kg/day (M); 2-yr chronic toxicity/carcinogenicity study, rats, diet, 5, 20, 80 mg/kg/day, anomalies of the testes and seminal vesicles, NOAEL = 5 mg/kg/day (M)
Developmental Effects	Moderate; Developmental toxicity study, gavage, rats, gd 6-15, 25, 100, 400 mg/kg/day, increased resorptions, decreased fetal viability, weight, and length, NOAEL = 100 mg/kg/day. Developmental toxicity study, gavage, rats, gd 7-19, 25, 50, 100, 200, 400 mg/kg/day, decreased fetal viability, NOAEL = 200 mg/kg/kday (M).
Immune System Effects	Low; Uncertain concern for immunotoxicity because substance is potentially an alkylating agent; Immunotoxicity assay, subcutaneous, mouse, 4 consecutive days, 0.25, 2.5, 25 mg/kg/day; lymphoid depletion of thymus, reduced responses to T-cell & B-cell antigens, NOAEL 0.25 mg/kg/day (M)
Neurotoxicity	Low; Acute delayed neurotoxicity study, hens, gavage, , no significant inhibition of brain neurotoxic esterase (NTE) activity at 10,000 mg/kg; 90-d study, hens, gavage, no behavioral effects or histopathological changes indicative of neurotoxicity, NOAEL = 100 mg/kg/day; In developmental toxicity assay, rats, gavage gd 7-19, no adverse effect on postnatal neurobehavioral tests of sensory and motor function, NOAEL = 200 mg/kg/day (M)
Genotoxicity/ Mutagenicity	Moderate; Positive, mutagenicity, *Salmonella*, with metabolic activation; Negative, mutagenicity, mouse lymphoma cells with or without activation & hamster lung cells with activation, *in vitro*; Negative, sex-linked recessive lethal, *Drosophila in vivo* (M) Positive only with activation, chromosomal aberrations, *in vitro*, human lymphocytes (MC) & mouse lymphoma cells (M); Negative, chromosomal aberrations, *in vitro,* Chinese hamster ovary cells (MC); Negative, sister chromatid exchange, *in vitro*, cell line not reported (MC); Positive with or without activation, sister chromatid exchange, *in vitro,* mouse lymphoma cell; Negative, chromosomal aberrations, *in vivo*, mice (M)
Systemic Effects	Moderate; 2-yr chronic toxicity/carcinogenicity study, rats, diet, 5, 20, 80 mg/kg/day, increased mortality, decreased body weight, anemia, anomalies of the liver, kidneys, testes, seminal vesicles, renal cortex, and adrenal cortex, LOAEL = 5 mg/kg/day. Inadequate 90-day dietary study, mice, 0.01, 0.04, 0.13, 0.42 and 1.33% in diet; increased mortality, decreased body weight, anemia, increased liver & kidney weight, liver histopathology; NOAEL= 0.01% dietary level (M)

Record ID: Proprietary A: Chloroalkyl phosphate (1)		**CAS No.**
Overall Hazard Concern for Non-Cancer Health Effects		MODERATE

4.2.6 Proprietary B

Record ID: Proprietary B: Aryl phosphate			**CAS No.**
			MW:
			MF:
			Physical Forms: **Neat:** Solid **As Formulated:** Liquid
			Use: Flame retardant, additive
SMILES:			
Name: Aryl phosphate			
Synonyms:			

ASSESSMENT SUMMARY:			
Concern Level	**HIGH**	**MODERATE**	**LOW**
Persistence			**X**
Bioconcentration		**X**	
Cancer Health Hazard			**X**
Non-Cancer Health Hazard		**X**	
Aquatic Toxicity Hazard	**X**		
Is the chemical predicted to be a PBT by PBT Profiler?	**No**		
Overall Hazard Concern	**Human Health Hazard: Moderate** **Aquatic Hazard: High**		

Record ID: Proprietary B: Aryl phosphate	CAS No.
PHYSICAL/CHEMICAL PROPERTIES	
Melting Point (deg C)	90 (E)
Boiling Point (deg C)	>400 (E)
Boiling Point Pressure (mm Hg)	760 (E)
Vapor Pressure (mm Hg)	$<10^{-6}$ (E)
Water Solubility (g/L)	$<10^{-6}$ (E)
Log K_{ow}	6.16 (E)
ENVIRONMENTAL TRANSPORT AND FATE:	
Transport	
Henry's Law Constant – HLC	$7.74x10^{-8}$ atm-m^3/mole (E)
Soil Adsorption Coefficient – K_{oc}	$2.6x10^4$ (E)
Bioconcentration Factor – BCF	1820 (E)
Persistence	
Experimental Biodeg Tests	46% ThOD after 28 days in OECD 301F (MC)
Ultimate Biodeg Model	Weeks -months (E)
Primary Biodeg Model	Days-weeks (E)
BOD or COD	
Atmospheric Half-life	9.3 hours (E)
Hydrolysis Half-life	
Volatilization Half-life for Model River	605 days (E)
Volatilization Half-life for Model Lake	Negligible (E)
Removal in Sewage Treatment Plant	93% (E)
Ready Biodegradability	Not ready biodegradable (MC)
Byproducts	
Degradation Products	
Metabolites	

Record ID: Proprietary B: Aryl phosphate		**CAS No.**
ECOTOXICITY:		
ECOSAR Class	Ester-phosphate	
Acute Toxicity		
Fish LC_{50}	96-h LC50, NES (No effects at saturation) (E)	
Daphnid LC_{50}	48-h LC50, NES (E) 48-h EC50, > 0.77 mg/L (MC) 48-h NOEC, ≥ 0.77 mg/L (MC)	
Green Algae EC_{50}	96-h EC50, NES (E) 72-h EC50 (Growth inhibition), approx. 0.480 mg/L (MC)	
Chronic Toxicity		
Fish ChV	NES (E)	
Daphnid ChV	NES (E)	
Green Algae ChV	NES (E)	
Overall Hazard Concern for Aquatic Toxicity	HIGH (chronic toxicity and only when 1 or 2 isopropyls are present)	
HEALTH EFFECTS:		
Absorption	Nil thru skin as neat solid; poor thru skin when in solution; poor thru lungs and GI tract by analogy to closely related compounds (P)	
CANCER HEALTH EFFECTS:		
Experimental data		
OncoLogic Results	Marginal (E)	
Overall Hazard Concern for Carcinogenicity	LOW	

Record ID: Proprietary B: Aryl phosphate	CAS No.
NON-CANCER HEALTH EFFECTS:	
Acute Toxicity	Low in mixtures; Rat oral LD_{50} >5000 mg/kg (no deaths), >20,000 mg/kg (4/10 deaths); Rat 1-hr inhalation LC_{50} > 200 mg/L; Rat dermal LD_0 > 2000 mg/kg (no deaths)(M)
Eye Irritation	Moderate in mixtures; Rabbits, very slight eye irritation (M)
Skin Irritation	Low in mixtures; Not irritating to intact or abraded skin in rabbits (M)
Skin Sensitizer	Low by analogy to a closely related compound (P)
Reproductive Effects	Preliminary results of an unfinished 39-41-day combined subchronic plus reproductive/developmental toxicity screening test suggest that the reproductive hazard may be moderate, rat, oral gavage, ovarian weight effect at ≥25 mg/kg/day, epididymal weight effect and reduced fertility at 100 and 400 mg/kg/day (MC)
Developmental Effects	Preliminary results of an unfinished 39-41-day combined subchronic plus reproductive/developmental toxicity screening test suggests the developmental hazard may be moderate; rat, oral gavage, reduced pre- and post-natal survival at 400 mg/kg/day (MC)
Immune System Effects	
Neurotoxicity	Moderate in mixtures; acute delayed neurotoxicity assay, hens, oral gavage, NOAEL = 12 mg/kg/day for neurotoxic esterase (NTE) inhibition, LOAEL = 1000 mg/kg/day; delayed oral neurotoxicity, hens, 2 oral treatments 3 weeks apart, transient dose-related gait impairment (LOAEL = 12 mg/kg/day), but no neurohistopathology at doses as high as 11,700 mg/kg/day (M); Also by analogy to closely related compounds and professional judgment; neurotoxicity study, hens, oral gavage, 3, 5, 7, 9 g/kg, ataxia, neuropathological lesions, LOAEL = 3000 mg/kg; neurotoxicity study, hens, oral gavage, 10, 20, 90, 270 mg/kg/day, ataxia, nerve degeneration, NOAEL = 20 mg/kg/day; NTE inhibition (M,P)
Genotoxicity/Mutagenicity	Low by analogy to a closely related compound; Negative, Ames assay (P)
Systemic Effects	Moderate in mixture (liver effects); 28-d repeated-dose study (inadequate), rats, diet, 0.1%, 0.5%, 1.0%, liver effects all doses, LOAEL = 0.1% (M); Preliminary results of an unfinished a 39-41-day combined subchronic toxicity with reproductive/developmental screening test suggest that there may be a moderate hazard for subchronic toxicity (adrenal and liver effects), rat, oral gavage, adrenal weight effect in females, LOAEL = 25 mg/kg/day (MC)

Record ID: Proprietary B: Aryl phosphate		**CAS No.**
Overall Hazard Concern for Non-Cancer Health Effects	MODERATE	

4.2.7 Proprietary C

Record ID: Proprietary C: Chloroalkyl phosphate (2)	**CAS No.**
	MW:
	MF:
	Physical Forms: **Neat:** Solid **As Formulated:** Liquid
	Use: Flame retardant, additive
SMILES:	
Name: Chloroalkyl phosphate (2)	
Synonyms:	

ASSESSMENT SUMMARY:

Concern Level	HIGH	MODERATE	LOW
Persistence			
Bioconcentration			**X**
Cancer Health Hazard		**X**	
Non-Cancer Health Hazard		**X**	
Aquatic Toxicity Hazard		**X**	
Is the chemical predicted to be a PBT by PBT Profiler?	**No**		
Overall Hazard Concern	**Human Health Hazard: Moderate** **Aquatic Hazard: Moderate**		

Record ID: Proprietary C: Chloroalkyl phosphate (2)	CAS No.
PHYSICAL/CHEMICAL PROPERTIES	
Melting Point (deg C)	< 20 (P)
Boiling Point (deg C)	>400 (E)
Boiling Point Pressure (mm Hg)	760 (E)
Vapor Pressure (mm Hg)	$<10^{-6}$ (E)
Water Solubility (g/L)	0.0028 (E)
Log K_{ow}	4.29 (E)
ENVIRONMENTAL TRANSPORT AND FATE:	
Transport	
Henry's Law Constant – HLC	$2.74x10^{-14}$ atm-m^3/mole (E)
Soil Adsorption Coefficient – K_{oc}	1.1X104 (MC); $6.07x10^6$ (E)
Bioconcentration Factor – BCF	6.64 (E)
Persistence	
Experimental Biodeg Tests	37% oxygen uptake after 28 days in OECD 302C (MC); 5% degradation in modified Sturm test, 28 days (MC); 8-15% inhibition to activated sludge (MC)
Ultimate Biodeg Model	Recalcitrant (E)
Primary Biodeg Model	Weeks (E)
BOD or COD	
Atmospheric Half-life	1.6 hours (E)
Hydrolysis Half-life	Preliminary results suggest that the half-life is greater than 1 year (MC)
Volatilization Half-life for Model River	Negligible (E)
Volatilization Half-life for Model Lake	Negligible (E)
Removal in Sewage Treatment Plant	44.7% (E)
Ready Biodegradability	Not ready biodegradable (MC)
Byproducts	
Degradation Products	
Metabolites	

Record ID: Proprietary C: Chloroalkyl phosphate (2)	CAS No.
ECOTOXICITY:	
ECOSAR Class	Ester-phosphate
Acute Toxicity	
Fish LC_{50}	96-h LC50, 9.6 mg/L (E) 96-h LC50, 52.2 mg/L (MC)
Daphnid LC_{50}	48-h EC50, 30.0 mg/L (E) 48-h EC50, 41.9 mg/L (MC)
Green Algae EC_{50}	96-h EC50, 1.5 mg/L (E) 96-h EC50 (growth rate inhibition), 38.5 mg/L (MC) 96-h EC50 (growth inhibition), 20.1 mg/L (MC)
Chronic Toxicity	
Fish ChV	1.0 mg/L (E)
Daphnid ChV	3.0 mg/L, (E) 23-d EC50 (parental mortality), 7.31 mg/L (MC) LOEC (impaired reproduction), > 3.68 mg/L (MC) NOEC (impaired reproduction), ≥ 3.68 mg/L (MC)
Green Algae ChV	1.2 mg/L (E)
Overall Hazard Concern for Aquatic Toxicity	MODERATE
HEALTH EFFECTS:	
Absorption	Poor absorption via all routes (P)
CANCER HEALTH EFFECTS:	
Experimental data	Moderate by analogy to a closely related compound; 2-yr chronic toxicity/carcinogenicity study, rats, diet, 5, 20, 80 mg/kg/day, increased benign adrenal cortex tumors and hepatocellular adenomas at 20 and 80 mg/kg/day (P)
OncoLogic Results	Low-moderate (E)
Overall Hazard Concern for Carcinogenicity	MODERATE
NON-CANCER HEALTH EFFECTS:	
Acute Toxicity	Low; Rat oral LD_{50} between 2000 and 5000 mg/kg (M), >2000 mg/kg (MC); Rat inhalation LC_{50} >1.65 mg/L (no death) (MC); Rat dermal LD_{50} > 2000 mg/kg (no deaths or clinical signs)(M, MC)
Eye Irritation	Moderate; Slight eye (conjunctival) irritation (M, MC)
Skin Irritation	Moderate, rabbits; No skin irritation (M); slight irritation (erythema) (MC); mild irritation (erythema, edema) (MC)

Record ID: Proprietary C: Chloroalkyl phosphate (2)	**CAS No.**
Skin Sensitizer	Moderate; guinea pig, no sensitization (M), mild sensitization (MC)
Reproductive Effects	A 4-wk oral gavage study in rats reported no histopathology of reproductive organs in either sex at a NOAEL of 600 mg/kg/day, but the study duration was short (MC); Moderate by analogy to a closely related compound; 12-wk male reproduction study, rabbits, gavage, no effects on male fertility or spermatogenesis, NOAEL = 200 mg/kg/day; 2-yr chronic toxicity/carcinogenicity study, rats, diet, 5, 20, 80 mg/kg/day, anomalies of the testes and seminal vesicles, NOAEL = 5 mg/kg/day (P)
Developmental Effects	Moderate by analogy to closely related compound; Developmental toxicity study on one analog, gavage, rats, gd 6-15, 25, 100, 400 mg/kg/day, increased resorptions, decreased fetal viability, weight, and length, fetal NOAEL = 100 mg/kg/day (P); Developmental toxicity study on another analog, gavage, rats, 15, 50, 150, 500 mg/kg/day, maternal deaths at 150 mg/kg/day, maternal NOAEL = 50 mg/kg/day, fetal NOAEL = 15 mg/kg/day (P)
Immune System Effects	
Neurotoxicity	Low, neurotoxicity screening battery after 4-week oral gavage, rats, no behavioral effects or neurohistopathology, NOAEL = 600 mg/kg/day (MC). Also by analogy to a closely related compound; Acute study, hens, gavage, delayed neurotoxicity, no inhibition of brain neurotoxic esterase (NTE) activity, NOAEL = 10,000 mg/kg; 90-d study, hens, gavage, no behavioral effects or histopathological changes indicative of neurotoxicity, NOAEL = 100 mg/kg/day (P)
Genotoxicity/Mutagenicity	Low, Negative, mutagenicity in mouse lymphoma (M, MC) and Ames test (MC); Negative, chromosomal aberrations *in vitro* (human lymphocytes) (MC); Negative, bone marrow micronucleus assay in mice (oral gavage) (MC) Moderate for genotoxic effects other than mutagenicity by analogy to closely related compounds: Positive, chromosomal aberrations, *in vitro*, human lymphocytes; Positive, rat dominant lethal assay (P);

Record ID: Proprietary C: Chloroalkyl phosphate (2)		**CAS No.**
Systemic Effects	Moderate, 4-week oral gavage study, rats (liver effects), NOAEL = 15 mg/kg,day, LOAEL = 150 mg/kg/day (MC); Also by analogy to a closely related compound; 2-yr chronic toxicity/carcinogenicity study, rats, diet, 5, 20, 80 mg/kg/day, increased mortality, decreased body weight, anomalies of the liver, kidneys, testes, seminal vesicles, renal cortex, and adrenal cortex, NOAEL = 5 mg/kg/day (P)	
Overall Hazard Concern for Non-Cancer Health Effects	MODERATE	

4.2.8 Proprietary D

Record ID: Proprietary D: Reactive brominated flame retardant	**CAS No.**
	MW:
	MF:
	Physical Forms: **Neat:** Solid **As Formulated:** Liquid
	Use: Flame retardant, reactive
SMILES:	
Name: Reactive brominated flame retardant	
Synonyms:	

ASSESSMENT SUMMARY:			
Concern Level	**HIGH**	**MODERATE**	**LOW**
Persistence			**X**
Bioconcentration			**X**
Cancer Health Hazard			**X**
Non-Cancer Health Hazard		**X**	
Aquatic Toxicity Hazard		**X**	
Is the chemical predicted to be a PBT by PBT Profiler?	**No**		
Overall Hazard Concern	**Human Health Hazard: Moderate** **Aquatic Hazard: Moderate**		

Record ID: Proprietary D: Reactive brominated flame retardant	**CAS No.**
PHYSICAL/CHEMICAL PROPERTIES	
Melting Point (deg C)	< 20 (P)
Boiling Point (deg C)	>400 (E)
Boiling Point Pressure (mm Hg)	760 (E)
Vapor Pressure (mm Hg)	$<10^{-6}$ (E)
Water Solubility (g/L)	0.007 to 0.15 (E)
Log K_{ow}	3.83 (E)
ENVIRONMENTAL TRANSPORT AND FATE:	
Transport	
Henry's Law Constant – HLC	2.23×10^{-21} atm-m^3/mole (E)
Soil Adsorption Coefficient – K_{oc}	10 (E)
Bioconcentration Factor – BCF	39 (E)
Persistence	
Experimental Biodeg Tests	
Ultimate Biodeg Model	Months (E)
Primary Biodeg Model	Weeks (E)
BOD or COD	
Atmospheric Half-life	4.2 hours (E)
Hydrolysis Half-life	
Volatilization Half-life for Model River	Negligible (E)
Volatilization Half-life for Model Lake	Negligible (E)
Removal in Sewage Treatment Plant	23% (E)
Ready Biodegradability	Not ready biodegradable (E)
Byproducts	
Degradation Products	
Metabolites	

Record ID: Proprietary D: Reactive brominated flame retardant	CAS No.
ECOTOXICITY:	
ECOSAR Class	Ester-phthalate
Acute Toxicity	
Fish LC_{50}	96-h LC50, ≤ 67.0 mg/L (E)
Daphnid LC_{50}	48-h LC50, ≤ 280.0 mg/L (E)
Green Algae EC_{50}	96-h EC50, ≤ 5.4 mg/L (E)
Chronic Toxicity	
Fish ChV	≤ 7.0 mg/L (E)
Daphnid ChV	≤ 30.0 mg/L (E)
Green Algae ChV	≤ 4.2 mg/L (E)
Overall Hazard Concern for Aquatic Toxicity	MODERATE
HEALTH EFFECTS:	
Absorption	Poor all routes (P)
CANCER HEALTH EFFECTS:	
Experimental data	
OncoLogic Results	Marginal (E)
Overall Hazard Concern for Carcinogenicity	LOW

Record ID: Proprietary D: Reactive brominated flame retardant	**CAS No.**
NON-CANCER HEALTH EFFECTS:	
Acute Toxicity	Low; Rat oral LD_{50} >10,000 mg/kg (no deaths); Rabbit dermal LD_{50} >20,000 mg/kg (no deaths); Rat 1-hr inhalation LC_{50} >0.008 mg/L (no deaths) (M); Low by analogy to a closely related compound; Rat oral LD_{50} = 2874 (P)
Eye Irritation	Moderate, mild reversible conjunctival irritant or not an eye irritant in rabbits (M)
Skin Irritation	Low, not an irritant to intact skin, mild reversible irritation of abraded skin in rabbits (M)
Skin Sensitizer	Moderate by analogy to a closely related compound (P)
Reproductive Effects	
Developmental Effects	
Immune System Effects	
Neurotoxicity	Moderate by analogy to a closely related compound: Acute oral study, rats, brain hemorrhages (P)
Genotoxicity/Mutagenicity	Low, Negative in Ames assay with or without metabolic activation (M); Low also by analogy to a closely related compound; Negative in Ames assay (P)
Systemic Effects	Moderate by analogy to closely related compounds: 28-d, rats, oral, 160, 400, 1000 mg/kg/day, renal effects at all doses; 21-d repeated-dose study, rats, inhalation, 2-8 mg/L, adrenal, thyroid, lung, and liver effects; 28-d repeated-dose study, rabbits, dermal, 5000 mg/kg, kidney, liver, blood effects (P)
Overall Hazard Concern for Non-Cancer Health Effects	MODERATE

4.2.9 Proprietary E

Record ID: Proprietary E: Tetrabromophthalate diol diester			**CAS No.**
			MW:
			MF:
			Physical Forms: **Neat:** Solid **As Formulated:** Liquid
			Use: Flame retardant, additive
SMILES:			
Name: Tetrabromophthalate diol diester			
Synonyms:			
ASSESSMENT SUMMARY:			
Concern Level	**HIGH**	**MODERATE**	**LOW**
Persistence	**X**		
Bioconcentration			**X**
Cancer Health Hazard			**X**
Non-Cancer Health Hazard		**X**	
Aquatic Toxicity Hazard			
Is the chemical predicted to be a PBT by PBT Profiler?	**No**		
Overall Hazard Concern	**Human Health Hazard: Moderate** **Aquatic Hazard:**		

Record ID: Proprietary E: Tetrabromophthalate diol diester		**CAS No.**
PHYSICAL/CHEMICAL PROPERTIES		
Melting Point (deg C)	< 20 (P)	
Boiling Point (deg C)	>400 (P)	
Boiling Point Pressure (mm Hg)	760	
Vapor Pressure (mm Hg)	$<10^{-6}$ (P)	
Water Solubility (g/L)	0.002 to $<10^{-6}$ (P)	
Log K_{ow}	5.7 (E)	
ENVIRONMENTAL TRANSPORT AND FATE:		
Transport		
Henry's Law Constant – HLC	$<10^{-8}$ atm-m^3/mole (P)	
Soil Adsorption Coefficient – K_{oc}		
Bioconcentration Factor – BCF	Low (P)	
Persistence		
Experimental Biodeg Tests		
Ultimate Biodeg Model		
Primary Biodeg Model		
BOD or COD		
Atmospheric Half-life		
Hydrolysis Half-life		
Volatilization Half-life for Model River	Negligible (P)	
Volatilization Half-life for Model Lake	Negligible (P)	
Removal in Sewage Treatment Plant	50-90 (P)	
Ready Biodegradability	Not Ready Biodegradable (P)	
Byproducts		
Degradation Products		
Metabolites		

Record ID: Proprietary E: Tetrabromophthalate diol diester	**CAS No.**
ECOTOXICITY:	
ECOSAR Class	Ester-phthalate
Acute Toxicity	
Fish LC_{50}	96-h LC50, NES (No effects at saturation) (E)
Daphnid LC_{50}	48-h LC50, NES (E)
Green Algae EC_{50}	96-h EC50, NES (E)
Chronic Toxicity	
Fish ChV	0.040 or NES (E)
Daphnid ChV	0.030 or NES (E)
Green Algae ChV	0.100 or NES (E)
Overall Hazard Concern for Aquatic Toxicity	HIGH (chronic toxicity only)
HEALTH EFFECTS:	
Absorption	Absorption of LMW fraction is expected to be poor by all routes based on physicochemical properties (P)
CANCER HEALTH EFFECTS:	
Experimental data	
OncoLogic Results	Cannot be run in OncoLogic
Overall Hazard Concern for Carcinogenicity	LOW

Record ID: Proprietary E: Tetrabromophthalate diol diester	CAS No.
NON-CANCER HEALTH EFFECTS:	
Acute Toxicity	
Eye/Skin Irritation	
Skin Sensitizer	
Reproductive Effects	
Developmental Effects	
Immune System Effects	
Neurotoxicity	
Genotoxicity/Mutagenicity	
Systemic Effects	Moderate by analogy to closely related compounds; kidney toxicity, NOAEL = 400 mg/kg (M); liver toxicity based on brominated phenyl moiety (P)
Overall Hazard Concern for Non-Cancer Health Effects	MODERATE

4.2.10 Proprietary F

Record ID: Proprietary F: Halogenated aryl ester			**CAS No.**
			MW:
			MF:
			Physical Forms: **Neat:** Liquid **As Formulated:**
			Use: Flame retardant, additive
SMILES:			
Name: Halogenated aryl ester			
Synonyms:			
ASSESSMENT SUMMARY:			
Concern Level	**HIGH**	**MODERATE**	**LOW**
Persistence			**X**
Bioconcentration			**X**
Cancer Health Hazard			**X**
Non-Cancer Health Hazard		**X**	
Aquatic Toxicity Hazard	**X**		
Is the chemical predicted to be a PBT by PBT Profiler?	**No**		
Overall Hazard Concern	**Human Health Hazard: Moderate** **Aquatic Hazard: Low**		

Record ID: Proprietary F: Halogenated aryl ester	**CAS No.**
PHYSICAL/CHEMICAL PROPERTIES	
Melting Point (deg C)	< 20 (P)
Boiling Point (deg C)	>400 (E)
Boiling Point Pressure (mm Hg)	760 (E)
Vapor Pressure (mm Hg)	$<1x10^{-6}$ (E)
Water Solubility (g/L)	$<1x10^{-6}$ (E)
Log Kow	8.75 (E)
ENVIRONMENTAL TRANSPORT AND FATE:	
Transport	
Henry's Law Constant – HLC	7.05 $x10^{-6}$ atm-m^3/mole (E)
Soil Adsorption Coefficient – K_{oc}	>28,840 (M)
Bioconcentration Factor – BCF	1.7-6.2 (M)
Persistence	
Experimental Biodeg Tests	3.5 days in water shake flask die-away test, 8.5 days in sediment (M); 6% biodegradation after 28 days in closed bottle test (M)
Ultimate Biodeg Model	Months (E)
Primary Biodeg Model	Weeks (E)
BOD or COD	
Atmospheric Half-life	12 hours (E)
Hydrolysis Half-life	>1 year @ pH 4, 7, and 9 (M)
Volatilization Half-life for Model River	8 days (E)
Volatilization Half-life for Model Lake	98 days (E)
Removal in Sewage Treatment Plant	90% (E)
Ready Biodegradability	Not ready biodegradable (E)
Byproducts	
Degradation Products	
Metabolites	

Record ID: Proprietary F: Halogenated aryl ester		**CAS No.**
ECOTOXICITY:		
ECOSAR Class	Esters	
Acute Toxicity		
Fish LC_{50}	96 hr LC50, 12 mg/L (M)	
Daphnid LC_{50}	24 hr EC50, 1.2 mg/L; 48 hr EC50, 0.42 mg/L (M)	
Green Algae EC_{50}	96 hr EC50, >5.1 mg/L (M)	
Chronic Toxicity		
Fish ChV	No effect at saturation (E)	
Daphnid ChV	No effect at saturation (E)	
Green Algae ChV	No effect at saturation (E)	
Overall Hazard Concern for Aquatic Toxicity	HIGH	
HEALTH EFFECTS:		
Absorption	Poor absorption via all routes (P)	
CANCER HEALTH EFFECTS:		
Experimental data	Uncertain by analogy to a closely related chemical classes (P)	
OncoLogic Results		
Overall Hazard Concern for Carcinogenicity	LOW	

Record ID: Proprietary F: Halogenated aryl ester	**CAS No.**
NON-CANCER HEALTH EFFECTS:	
Acute Toxicity	Low; Rat oral LD50 >2000 mg/kg (M)
Eye Irritation	
Skin Irritation	
Skin Sensitizer	
Reproductive Effects	Moderate by analogy to a closely related compound (P)
Developmental Effects	Moderate by analogy to a closely related compound (P)
Immune System Effects	
Neurotoxicity	
Genotoxicity/Mutagenicity	
Systemic Effects	Moderate concern for liver effects by analogy to a closely related compound (P)
Overall Hazard Concern for Non-Cancer Health Effects	MODERATE

4.2.11 Proprietary G

Record ID: Proprietary G: Triaryl phosphate, isopropylated	**CAS No.**
	MW:
	MF:
	Physical Forms: **Neat:** Solid **As Formulated:** Liquid
	Use: Flame retardant, additive
SMILES:	
Name: Triaryl phosphate, isopropylated	
Synonyms:	

ASSESSMENT SUMMARY:

Concern Level	HIGH	MODERATE	LOW
Persistence			X
Bioconcentration		X	
Cancer Health Hazard			X
Non-Cancer Health Hazard		X	
Aquatic Toxicity Hazard	X		
Is the chemical predicted to be a PBT by PBT Profiler?	No		
Overall Hazard Concern	Human Health Hazard: Moderate Aquatic Hazard: High		

Record ID: Proprietary G: Triaryl phosphate, isopropylated	CAS No.
PHYSICAL/CHEMICAL PROPERTIES	
Melting Point (deg C)	90 (E)
Boiling Point (deg C)	>400 (E)
Boiling Point Pressure (mm Hg)	760 (E)
Vapor Pressure (mm Hg)	$<10^{-6}$ (E)
Water Solubility (g/L)	$<10^{-6}$ (E)
Log K_{ow}	6.16 (E)
ENVIRONMENTAL TRANSPORT AND FATE:	
Transport	
Henry's Law Constant – HLC	7.74×10^{-8} atm-m^3/mole (E)
Soil Adsorption Coefficient – K_{oc}	2.6×10^{4} (E)
Bioconcentration Factor – BCF	1820 (E)
Persistence	
Experimental Biodeg Tests	46% ThOD after 28 days in OECD 301F (MC)
Ultimate Biodeg Model	Weeks -months (E)
Primary Biodeg Model	Days-weeks (E)
BOD or COD	
Atmospheric Half-life	9.3 hours (E)
Hydrolysis Half-life	
Volatilization Half-life for Model River	605 days (E)
Volatilization Half-life for Model Lake	Negligible (E)
Removal in Sewage Treatment Plant	93% (E)
Ready Biodegradability	Not ready biodegradable (MC)
Byproducts	
Degradation Products	
Metabolites	

Record ID: Proprietary G: Triaryl phosphate, isopropylated		CAS No.
ECOTOXICITY:		
ECOSAR Class	Ester-phosphate	
Acute Toxicity		
Fish LC_{50}	96-h LC50, NES (No effects at saturation) (E)	
Daphnid LC_{50}	48-h LC50, NES (E) 48-h EC50, > 0.77 mg/L (MC) 48-h NOEC, ≥ 0.77 mg/L (MC)	
Green Algae EC_{50}	96-h EC50, NES (E) 72-h EC50 (Growth inhibition), approx. 0.480 mg/L (MC)	
Chronic Toxicity		
Fish ChV	NES (E)	
Daphnid ChV	NES (E)	
Green Algae ChV	NES (E)	
Overall Hazard Concern for Aquatic Toxicity	HIGH (chronic toxicity and only when 1 or 2 isopropyls are present)	
HEALTH EFFECTS:		
Absorption	Nil thru skin as neat solid; poor thru skin when in solution; poor thru lungs and GI tract by analogy to closely related compounds (P)	
CANCER HEALTH EFFECTS:		
Experimental data		
OncoLogic Results	Marginal (E)	
Overall Hazard Concern for Carcinogenicity	LOW	

Record ID: Proprietary G: Triaryl phosphate, isopropylated	CAS No.
NON-CANCER HEALTH EFFECTS:	
Acute Toxicity	Low in mixtures; Rat oral LD_{50} >5000 mg/kg (no deaths), >20,000 mg/kg (4/10 deaths); Rat 1-hr inhalation LC_{50} > 200 mg/L; Rat dermal LD_0 > 2000 mg/kg (no deaths)(M)
Eye Irritation	Moderate in mixtures; Rabbits, very slight eye irritation (M)
Skin Irritation	Low in mixtures; Not irritating to intact or abraded skin in rabbits (M)
Skin Sensitizer	Low by analogy to a closely related compound (P)
Reproductive Effects	Preliminary results of an unfinished 39-41-day combined subchronic plus reproductive/developmental toxicity screening test suggest that the reproductive hazard may be moderate, rat, oral gavage, ovarian weight effect at ≥25 mg/kg/day, epididymal weight effect and reduced fertility at 100 and 400 mg/kg/day (MC)
Developmental Effects	Preliminary results of an unfinished 39-41-day combined subchronic plus reproductive/developmental toxicity screening test suggests the developmental hazard may be moderate; rat, oral gavage, reduced pre- and post-natal survival at 400 mg/kg/day (MC)
Immune System Effects	
Neurotoxicity	Moderate in mixtures; acute delayed neurotoxicity assay, hens, oral gavage, NOAEL = 12 mg/kg/day for neurotoxic esterase (NTE) inhibition, LOAEL = 1000 mg/kg/day; delayed oral neurotoxicity, hens, 2 oral treatments 3 weeks apart, transient dose-related gait impairment (LOAEL = 12 mg/kg/day), but no neurohistopathology at doses as high as 11,700 mg/kg/day (M); Also by analogy to closely related compounds and professional judgment; neurotoxicity study, hens, oral gavage, 3, 5, 7, 9 g/kg, ataxia, neuropathological lesions, LOAEL = 3000 mg/kg; neurotoxicity study, hens, oral gavage, 10, 20, 90, 270 mg/kg/day, ataxia, nerve degeneration, NOAEL = 20 mg/kg/day; NTE inhibition (M,P)
Genotoxicity/Mutagenicity	Low by analogy to a closely related compound; Negative, Ames assay (P)
Systemic Effects	Moderate in mixture (liver effects); 28-d repeated-dose study (inadequate), rats, diet, 0.1%, 0.5%, 1.0%, liver effects all doses, LOAEL = 0.1% (M); Preliminary results of an unfinished a 39-41-day combined subchronic toxicity with reproductive/developmental screening test suggest that there may be a moderate hazard for subchronic toxicity (adrenal and liver effects), rat, oral gavage, adrenal weight effect in females, LOAEL = 25 mg/kg/day (MC)

Record ID: Proprietary G: Triaryl phosphate, isopropylated		**CAS No.**
Overall Hazard Concern for Non-Cancer Health Effects	MODERATE	

4.2.12 Proprietary H

Record ID: Proprietary H: Halogenated aryl ester	**CAS No.**
	MW:
	MF:
	Physical Forms: **Neat:** Liquid **As Formulated:**
	Use: Flame retardant, additive
SMILES:	
Name: Halogenated aryl ester	
Synonyms:	

ASSESSMENT SUMMARY:

Concern Level	HIGH	MODERATE	LOW
Persistence			**X**
Bioconcentration			**X**
Cancer Health Hazard			**X**
Non-Cancer Health Hazard		**X**	
Aquatic Toxicity Hazard-	**X**		
Is the chemical predicted to be a PBT by PBT Profiler?	**No**		
Overall Hazard Concern	**Human Health Hazard: Moderate** **Aquatic Hazard: Low**		

Record ID: Proprietary H: Halogenated aryl ester	**CAS No.**
PHYSICAL/CHEMICAL PROPERTIES	
Melting Point (deg C)	< 20 (P)
Boiling Point (deg C)	>400 (E)
Boiling Point Pressure (mm Hg)	760 (E)
Vapor Pressure (mm Hg)	$<1x10^{-6}$ (E)
Water Solubility (g/L)	$<1x10^{-6}$ (E)
Log K_{ow}	12.0 (E)
ENVIRONMENTAL TRANSPORT AND FATE:	
Transport	
Henry's Law Constant – HLC	$3.08x10^{-7}$ atm-m^3/mole (E)
Soil Adsorption Coefficient – K_{oc}	>28,840 (M)
Bioconcentration Factor – BCF	1.7-6.2 (M)
Persistence	
Experimental Biodeg Tests	3.5 days in water shake flask die-away test, 8.5 days in sediment (M); 6% biodegradation after 28 days in closed bottle test (M)
Ultimate Biodeg Model	Months (E)
Primary Biodeg Model	Weeks (E)
BOD or COD	
Atmospheric Half-life	6 hours (E)
Hydrolysis Half-life	>1 year @ pH 4, 7, and 9 (M)
Volatilization Half-life for Model River	211 days (E)
Volatilization Half-life for Model Lake	2310 days (E)
Removal in Sewage Treatment Plant	90% (E)
Ready Biodegradability	Not ready biodegradable (E)
Byproducts	
Degradation Products	
Metabolites	

Record ID: Proprietary H: Halogenated aryl ester	**CAS No.**
ECOTOXICITY:	
ECOSAR Class	Esters
Acute Toxicity	
Fish LC_{50}	96 hr LC50, 12 mg/L (M)
Daphnid LC_{50}	24 hr EC50, 1.2 mg/L; 48 hr EC50, 0.42 mg/L (M)
Green Algae EC_{50}	96 hr EC50, >5.1 mg/L (M)
Chronic Toxicity	
Fish ChV	No effect at saturation (E)
Daphnid ChV	No effect at saturation (E)
Green Algae ChV	No effect at saturation (E)
Overall Hazard Concern for Aquatic Toxicity	HIGH
HEALTH EFFECTS:	
Absorption	Poor absorption via all routes (P)
CANCER HEALTH EFFECTS:	
Experimental data	Uncertain by analogy to a closely related chemical classes (P)
OncoLogic Results	
Overall Hazard Concern for Carcinogenicity	LOW

Record ID: Proprietary H: Halogenated aryl ester	**CAS No.**
NON-CANCER HEALTH EFFECTS:	
Acute Toxicity	Low; Rat oral LD50 >2000 mg/kg (M)
Eye Irritation	
Skin Irritation	
Skin Sensitizer	
Reproductive Effects	Moderate by analogy to a closely related compound (P)
Developmental Effects	Moderate by analogy to a closely related compound (P)
Immune System Effects	
Neurotoxicity	
Genotoxicity/Mutagenicity	
Systemic Effects	Moderate concern for liver effects by analogy to a closely related compound (P)
Overall Hazard Concern for Non-Cancer Health Effects	MODERATE

4.2.13 Proprietary I

<table>
<tr><td colspan="2" rowspan="1">Record ID: Proprietary I: Organic phosphate ester</td><td colspan="2">CAS No.</td></tr>
<tr><td colspan="2" rowspan="4"></td><td colspan="2">MW:</td></tr>
<tr><td colspan="2">MF:</td></tr>
<tr><td colspan="2">Physical Forms:
Neat: Solid
As Formulated:</td></tr>
<tr><td colspan="2">Use: Flame retardant, additive</td></tr>
<tr><td colspan="4">SMILES:</td></tr>
<tr><td colspan="4">Name: Organic phosphate ester</td></tr>
<tr><td colspan="4">Synonyms:</td></tr>
</table>

ASSESSMENT SUMMARY:			
Concern Level	**HIGH**	**MODERATE**	**LOW**
Persistence	**X**		
Bioconcentration			**X**
Cancer Health Hazard			**X**
Non-Cancer Health Hazard		**X**	
Aquatic Toxicity Hazard	**X**		
Is the chemical predicted to be a PBT by PBT Profiler?	**Yes**		
Overall Hazard Concern	**Human Health Hazard: Moderate** **Aquatic Hazard: High**		

Record ID: Proprietary I: Organic phosphate ester	**CAS No**.
PHYSICAL/CHEMICAL PROPERTIES	
Melting Point (deg C)	< 20 (P)
Boiling Point (deg C)	480 (E)
Boiling Point Pressure (mm Hg)	> 300 (MC)
Vapor Pressure (mm Hg)	$<10^{-6}$ (MC)
Water Solubility (g/L)	$8x10^{-4}$ (MC,P)
Log K_{ow}	6.89 (E)
ENVIRONMENTAL TRANSPORT AND FATE:	
Transport	
Henry's Law Constant – HLC	$4.89x10^{-14}$ atm-m^3/mole (E)
Soil Adsorption Coefficient – K_{oc}	$5.0x10^7$ (E)
Bioconcentration Factor – BCF	245 (MC)
Persistence	
Experimental Biodeg Tests	2.3% degradation after 28 days MITI-II (MC); 30% in 28 days and 52% in 140 days - closed bottle test (MC)
Ultimate Biodeg Model	Months (E)
Primary Biodeg Model	Days (E)
BOD or COD	
Atmospheric Half-life	2.1 hours (E)
Hydrolysis Half-life	Half-life of 20 days at pH 9 and 25 deg C (MC)
Volatilization Half-life for Model River	Negligible (E)
Volatilization Half-life for Model Lake	Negligible (E)
Removal in Sewage Treatment Plant	94% (E)
Ready Biodegradability	Not Ready Biodegradable (MC)
Byproducts	
Degradation Products	

Record ID: Proprietary I: Organic phosphate ester	**CAS No.**
Metabolites	
ECOTOXICITY:	
ECOSAR Class	Ester-phosphate
Acute Toxicity	
Fish LC_{50}	96-h LC50, NES (No effects at saturation) (E) 96-h LC50, 0.205 mg/L (MC)
Daphnid LC_{50}	48-h LC50, NES (E) 48-h LC50, > 0.846 mg/L (MC)
Green Algae EC_{50}	96-h EC50, NES (E)
Chronic Toxicity	
Fish ChV	0.200 or NES (E) LOEC (reduced larval survival and growth), 0.088 mg/L (MC)
Daphnid ChV	0.070 or NES (E) LOEC (reduced reproduction and growth), 0.147 mg/L (MC)
Green Algae ChV	0.140 or NES (E)
Overall Hazard Concern for Aquatic Toxicity	HIGH (chronic toxicity only)
HEALTH EFFECTS:	
Absorption	Poor all routes by analogy to closely related compounds and physicochemical properties (P)
CANCER HEALTH EFFECTS:	
Experimental data	
OncoLogic Results	Marginal (E)
Overall Hazard Concern for Carcinogenicity	LOW

Record ID: Proprietary I: Organic phosphate ester	CAS No.
NON-CANCER HEALTH EFFECTS:	
Acute Toxicity	Low; rat oral LD_{50} > 5 g/kg; rabbit dermal LD_{50} > 5 g/kg; LC_{50}>1.55 mg/L (MC)
Eye Irritation	Moderate; mild and transient eye irritation, rabbits; no eye irritation, rabbits (MC)
Skin Irritation	Low; no skin irritation in rabbits (MC)
Skin Sensitizer	Low; no skin sensitization in guinea pigs (MC)
Reproductive Effects	Low; NOAEL>1000 mg/kg/day in reproductive/developmental screening test in rats (MC)
Developmental Effects	Low; NOAEL>1000 mg/kg/day in reproductive/developmental screening test in rats (MC)
Immune System Effects	
Neurotoxicity	Low by analogy to a closely related compound; 42-d neurotoxicity test, hens, NOAEL = 5 g/kg/day (P)
Genotoxicity/Mutagenicity	Low; Negative, mouse micronucleus assay, *in vivo*, i.p.; Negative, chromosomal aberrations *in vitro*; Negative Ames assay, *Salmonella* and *E. coli*; Negative mouse lymphoma assay (MC)
Systemic Effects	Moderate by analogy to a closely related compound; 28-d repeated-dose study, rat, oral gavage, slight liver toxicity, NOAEL = 300 mg/kg/day, LOAEL = 1000 mg/kg/day (P)
Overall Hazard Concern for Non-Cancer Health Effects	MODERATE

4.2.14 Proprietary J

Record ID: Proprietary J: Aryl phosphate	**CAS No.**
	MW:
	MF:
	Physical Forms: **Neat:** Liquid **As Formulated:**
	Use: Flame retardant, additive
SMILES:	
Name: Aryl phosphate	
Synonyms:	

ASSESSMENT SUMMARY:			
Concern Level	**HIGH**	**MODERATE**	**LOW**
Persistence			**X**
Bioconcentration			**X**
Cancer Health Hazard			**X**
Non-Cancer Health Hazard		**X**	
Aquatic Toxicity Hazard	**X**		
Is the chemical predicted to be a PBT by PBT Profiler?	**No**		
Overall Hazard Concern	**Human Health Hazard: Moderate** **Aquatic Hazard: High**		

Record ID: Proprietary J: Aryl phosphate	**CAS No.**
PHYSICAL/CHEMICAL PROPERTIES	
Melting Point (deg C)	-21 (M)
Boiling Point (deg C)	425 (M)
Boiling Point Pressure (mm Hg)	760 (M)
Vapor Pressure (mm Hg)	1.4×10^{-6} (M)
Water Solubility (g/L)	0.0032 (M)
Log K_{ow}	5.12 (M)
ENVIRONMENTAL TRANSPORT AND FATE:	
Transport	
Henry's Law Constant – HLC	8.48×10^{-7} atm-m^3/mole (E)
Soil Adsorption Coefficient – K_{oc}	3.7×10^{4} (E)
Bioconcentration Factor – BCF	290 (E)
Persistence	
Experimental Biodeg Tests	
Ultimate Biodeg Model	Weeks-months (E)
Primary Biodeg Model	Days-weeks (E)
BOD or COD	
Atmospheric Half-life	8.2 hours (E)
Hydrolysis Half-life	
Volatilization Half-life for Model River	54 days (E)
Volatilization Half-life for Model Lake	594 days (E)
Removal in Sewage Treatment Plant	81.2% (E)
Ready Biodegradability	Not ready biodegradable (E)
Byproducts	
Degradation Products	
Metabolites	

Record ID: Proprietary J: Aryl phosphate	**CAS No.**
ECOTOXICITY:	
ECOSAR Class	Ester-phosphate
Acute Toxicity	
Fish LC_{50}	96-h LC50, NES (No effects at saturation) (E)
Daphnid LC_{50}	48-h LC50, NES (E)
Green Algae EC_{50}	96-h EC50, 0.020 mg/L or NES (E)
Chronic Toxicity	
Fish ChV	0.003 mg/L (E)
Daphnid ChV	0.002 mg/L (E)
Green Algae ChV	0.020 mg/L (E)
Overall Hazard Concern for Aquatic Toxicity	HIGH (chronic toxicity only)
HEALTH EFFECTS:	
Absorption	Nil thru skin as neat solid; poor thru skin when in solution; poor thru lungs and GI tract by analogy to closely related compounds (P)
CANCER HEALTH EFFECTS:	
Experimental data	
OncoLogic Results	Marginal (E)
Overall Hazard Concern for Carcinogenicity	LOW

Record ID: Proprietary J: Aryl phosphate	**CAS No.**
NON-CANCER HEALTH EFFECTS:	
Acute Toxicity	Low; Rat oral LD_{50} > 5000 mg/kg; Rat dermal LD_{50} > 2000 mg/kg (M)
Eye Irritation	Low; Rabbits, no eye irritation (M)
Skin Irritation	Moderate; Rabbits, mild skin irritation (M)
Skin Sensitizer	Low by analogy to a closely related compound (P)
Reproductive Effects	Low, 90-day oral toxicity (diet), rats, no effect on histopathology or weights of reproductive organs in males or females, NOAEL = 1600 ppm (M)
Developmental Effects	
Immune System Effects	
Neurotoxicity	Low, delayed neurotoxicity; 5-d study, hens, oral gavage, 5000 mg/kg/day, no evidence of delayed neurotoxicity; 90-day oral toxicity (diet), rats, no neurohistopathology in males or females, NOAEL = 1600 ppm (M); Also by analogy to a closely related compound (P)
Genotoxicity/Mutagenicity	Studies on poorly defined mixtures suggest negative results for mutagenicity (*Salmonella typhimurium*, *Saccharomyces cerevisiae*, mouse lymphoma cells), chromosomal aberration *in vitro* (mouse lymphoma cells) and sister chromatid exchange *in vitro* (mouse lymphoma cells) (M)
Systemic Effects	Moderate, 90-day oral toxicity (diet), rats, increased absolute and relative liver weights (both sexes) and adrenal weights (females), relative kidney weights (males), NOAEL = 400 ppm, LOAEL = 1600 ppm (M); Also by analogy to closely related compounds (liver effects); 28-d repeated-dose study (inadequate), rats, diet, liver effects at 0.5%, NOAEL = 0.1% (P)
Overall Hazard Concern for Non-Cancer Health Effects	MODERATE

4.2.15 Proprietary K

Record ID: Proprietary K: Aryl phosphate	**CAS No.**
	MW:
	MF:
	Physical Forms: **Neat:** Solid **As Formulated:**
	Use: Flame retardant, additive
SMILES:	
Name: Aryl phosphate	
Synonyms:	

ASSESSMENT SUMMARY:			
Concern Level	**HIGH**	**MODERATE**	**LOW**
Persistence			**X**
Bioconcentration			**X**
Cancer Health Hazard			**X**
Non-Cancer Health Hazard		**X**	
Aquatic Toxicity Hazard			**X**
Is the chemical predicted to be a PBT by PBT Profiler?	**No**		
Overall Hazard Concern	**Human Health Hazard: Moderate** **Aquatic Hazard: Low**		

Record ID: Proprietary K: Aryl phosphate	**CAS No.**
PHYSICAL/CHEMICAL PROPERTIES	
Melting Point (deg C)	90 (E)
Boiling Point (deg C)	>400 (E)
Boiling Point Pressure (mm Hg)	760 (E)
Vapor Pressure (mm Hg)	$<10^{-6}$ (E)
Water Solubility (g/L)	$<10^{-6}$ (E)
Log K_{ow}	8.52 (E)
ENVIRONMENTAL TRANSPORT AND FATE:	
Transport	
Henry's Law Constant – HLC	$2.65x10^{-7}$ atm-m^3/mole (E)
Soil Adsorption Coefficient – K_{oc}	$2.7x10^5$ (E)
Bioconcentration Factor – BCF	89 (E)
Persistence	
Experimental Biodeg Tests	
Ultimate Biodeg Model	Months (E)
Primary Biodeg Model	Days-weeks (E)
BOD or COD	
Atmospheric Half-life	9.7 hours (E)
Hydrolysis Half-life	
Volatilization Half-life for Model River	193 days (E)
Volatilization Half-life for Model Lake	Negligible (E)
Removal in Sewage Treatment Plant	94% (E)
Ready Biodegradability	Not ready biodegradable (E)
Byproducts	
Degradation Products	
Metabolites	

Record ID: Proprietary K: Aryl phosphate		**CAS No.**
ECOTOXICITY:		
ECOSAR Class	Ester-phosphate	
Acute Toxicity		
Fish LC_{50}	96-h LC50, NES (No effects at saturation) (E)	
Daphnid LC_{50}	48-h LC50, NES (E)	
Green Algae EC_{50}	96-h EC50, NES (E)	
Chronic Toxicity		
Fish ChV	NES (E)	
Daphnid ChV	NES (E)	
Green Algae ChV	NES (E)	
Overall Hazard Concern for Aquatic Toxicity	LOW	
HEALTH EFFECTS:		
Absorption	Nil thru skin as neat solid; poor thru skin when in solution; poor thru lungs and GI tract by analogy to closely related compounds (P)	
CANCER HEALTH EFFECTS:		
Experimental data		
OncoLogic Results	Marginal (E)	
Overall Hazard Concern for Carcinogenicity	LOW	

Record ID: Proprietary K: Aryl phosphate		**CAS No.**
NON-CANCER HEALTH EFFECTS:		
Acute Toxicity		
Eye/Skin Irritation		
Skin Sensitizer	Low by analogy to a closely related compound (P)	
Reproductive Effects		
Developmental Effects		
Immune System Effects		
Neurotoxicity	Low by analogy to a closely related compound (P)	
Genotoxicity/Mutagenicity		
Systemic Effects	Moderate by analogy to closely related compounds (liver effects); 28-d repeated-dose study (inadequate), rats, diet, liver effects at 0.5%, NOAEL = 0.1% (P)	
Overall Hazard Concern for Non-Cancer Health Effects	MODERATE	

4.2.16 Proprietary L

Record ID: Proprietary L: Aryl phosphate			**CAS No.**
			MW:
			MF:
			Physical Forms: **Neat:** Solid **As Formulated:**
			Use: Flame retardant, additive
SMILES:			
Name: Aryl phosphate			
Synonyms:			
ASSESSMENT SUMMARY:			
Concern Level	**HIGH**	**MODERATE**	**LOW**
Persistence			**X**
Bioconcentration			**X**
Cancer Health Hazard			**X**
Non-Cancer Health Hazard		**X**	
Aquatic Toxicity Hazard			**X**
Is the chemical predicted to be a PBT by PBT Profiler?	**No**		
Overall Hazard Concern	**Human Health Hazard: Moderate** **Aquatic Hazard: Low**		

Record ID: Proprietary L: Aryl phosphate		**CAS No.**
PHYSICAL/CHEMICAL PROPERTIES		
Melting Point (deg C)	90 (E)	
Boiling Point (deg C)	>400 (E)	
Boiling Point Pressure (mm Hg)	760 (E)	
Vapor Pressure (mm Hg)	$<10^{-6}$ (E)	
Water Solubility (g/L)	$<10^{-6}$ (E)	
Log K_{ow}	10.43 (E)	
ENVIRONMENTAL TRANSPORT AND FATE:		
Transport		
Henry's Law Constant – HLC (atm-m^3/mole)	$6.85x10^{-7}$ (E)	
Soil Adsorption Coefficient – K_{oc}	$1.9x10^{6}$ (E)	
Bioconcentration Factor – BCF	3.1 (E)	
Persistence		
Experimental Biodeg Tests		
Ultimate Biodeg Model	Recalcitrant (E)	
Primary Biodeg Model	Weeks (E)	
BOD or COD		
Atmospheric Half-life	8.8 hours (E)	
Hydrolysis Half-life		
Volatilization Half-life for Model River	79 days (E)	
Volatilization Half-life for Model Lake	Negligible (E)	
Removal in Sewage Treatment Plant	94% (E)	
Ready Biodegradability	Not ready biodegradable (E)	
Byproducts		
Degradation Products		
Metabolites		

Record ID: Proprietary L: Aryl phosphate		**CAS No.**
ECOTOXICITY:		
ECOSAR Class	Esters-phosphate	
Acute Toxicity		
Fish LC_{50}	96-h LC50, NES (No effects at saturation) (E)	
Daphnid LC_{50}	48-h LC50, NES (E)	
Green Algae EC_{50}	96-h EC50, NES (E)	
Chronic Toxicity		
Fish ChV	NES (E)	
Daphnid ChV	NES (E)	
Green Algae ChV	NES (E)	
Overall Hazard Concern for Aquatic Toxicity	LOW	
HEALTH EFFECTS:		
Absorption	Nil thru skin as neat solid, poor thru skin in solution; poor thru lungs and GI tract, based on closely related analogs	
CANCER HEALTH EFFECTS:		
Experimental data		
OncoLogic Results	Marginal	
Overall Hazard Concern for Carcinogenicity	LOW	

Record ID: Proprietary L: Aryl phosphate		**CAS No.**
NON-CANCER HEALTH EFFECTS:		
Acute Toxicity		
Eye Irritation		
Skin Irritation		
Skin Sensitizer	Low, concern for sensitization by analogy to closely related compounds (P)	
Reproductive Effects		
Developmental Effects		
Immune System Effects		
Neurotoxicity	Low; Not neurotoxic by analogy to a closely related compound which yielded negative results in all reliable oral assays for delayed acute neurotoxicity in hens and subchronic neurobehavioral assays in rats (M); Proprietary L lacks structural motifs associated with neurotoxicity (P)	
Genotoxicity/ Mutagenicity		
Systemic Effects	Moderate, systemic effects by analogy to closely related compounds, including 28-d repeated-dose study (inadequate), rats, diet, liver effects at 0.5%, NOAEL = 0.1% (P)	
Overall Hazard Concern for Non-Cancer Health Effects	MODERATE	

5.0 CONSIDERATIONS FOR SELECTING A REPLACEMENT FOR PENTABDE

Multiple factors must be considered when selecting an appropriate chemical flame retardant. In addition to environmental considerations, the flame retardant's use cannot negatively affect the quality of the foam (either physical characteristics or aesthetics that would reduce its desirability in the market place). This is a concern because the chemical will be incorporated in large amounts that may have effects on the foam product (e.g., pentaBDE formulations can make up as much as 8 percent by weight of the final foam product and other flame-retardant formulations have been used at concentrations above 10 percent). Additionally, it must be practical to use the chemical during production and processing of the foam and furniture with existing equipment. Finally, the chemical cannot be cost prohibitive.

The Furniture Flame Retardancy Partnership recognizes the significance of proposing practical alternatives. Therefore, future case studies regarding cost and performance evaluations of the alternatives discussed in this report are being explored.

5.1 Positive Environmental Attributes

This section identifies a set of positive attributes that companies should consider when formulating or selecting a flame retardant, or flame-retarded raw materials (e.g., foam and textiles) that will meet or exceed existing flammability standards. While ensuring that fire-safety standards are met, the following environmentally desirable chemical characteristics and attributes, relevant to many flame-retardant chemicals, should be considered general "rules of thumb".

Aerobic Degradation

Biodegradation and incineration are both forms of aerobic degradation or aerobic oxidation of the chemical. Biodegradation is mediated by living organisms and generally slow compared to incineration which is abiotic on a rapid time line. Environmental oxidation can be an abiotic form of aerobic degradation which is generally very slow for most chemicals. Abiotic oxidative processes addressed here occur in the absence of light. For the purposes of this report, two categories of aerobic degradation are being discussed: biodegradation and incineration. Attributes and considerations associated with these categories are discussed in more detail below.

<u>Readily Biodegradable: Low Persistence</u>

Typically, the environmental profile of a chemical improves with its rate of biodegradation. According to the Organization for Economic Cooperation and Development (OECD), a chemical is readily biodegradable if, in a 28-day test, it biodegrades 60 percent or more within 10 days of the time when degradation first reaches 10 percent (70% for DOC-based tests). There are two main features of readily biodegradable substances. Hydrophobic components composed of unsaturated linear alkyl chains (straight chain carbon molecules) biodegrade more rapidly under aerobic conditions in sewage treatment plants and the environment than highly branched chains.

Also, hydrophobic and hydrophilic components that are linked by an easily biodegradable group like a carboxylic acid ester will separate the hydrophobe from the hydrophile during the first step through aerobic biodegradation (i.e., ester hydrolysis).

Keep in mind that while the rate of biodegradation is important, it is equally important to be aware of the byproducts formed through the degradation process. In some cases, the products of biodegradation might be more toxic and persistent than the parent compound.

Incineration: Consideration of Combustion Byproducts

A concern with chemicals introduced into foam products is the formation of hazardous combustion byproducts either during a residential fire or if the consumer product is ultimately disposed to an incinerator. For example, halogenated flame retardants have the potential to combine with other organic compounds during combustion and form halogenated dioxins and furans. The formation of other hazardous combustion byproducts should also be considered.

Low Bioaccumulation Potential and Low Bioavailability: High log K_{ow} (>8); Large Molecule

The ability of a chemical to accumulate is often measured by the bioconcentration factor (BCF). A high BCF indicates a high potential to bioaccumulate. Quantified, chemical-specific BCFs are often not available; however, this property can be estimated by correlating it with another readily-available parameter - the octanol-water partition coefficient (K_{ow}). In general, a log K_{ow} of 3.5 to 5 corresponds to BCFs of approximately 1,000 to 5,000 and represent a moderate to high bioaccumulation potential, respectively. Note that as the log K_{ow} increases above 8, the bioaccumulation potential decreases.

The potential for a molecule to be absorbed and harm an organism is less when the molecule is larger than a certain size. Molecules with the following characteristics are not available for passive uptake through the respiratory membranes of aquatic organisms: (a) molecules with hydrophilic components having large cross-sectional diameters, at least twice as large as hexabromobenzene (i.e., greater than 10 Å), or (b) neutral and anionic surfactants with molecular weights greater than 1,000 daltons. (Large diameters or high molecular weights will limit toxicity to surface effects only and will prevent systemic effects.)

In addition, high molecular weight molecules tend to be less volatile and therefore, may exhibit less of a potential for inhalation exposure to vapors during manufacturing and processing of foam and textiles.

Reactive Flame Retardants: Even if a chemical has the potential to bioaccumulate, the environmental concerns may be reduced or mitigated if the chemical permanently incorporated into a commercial product. In this case, the potential for exposure to the chemical is greatly decreased. Reactive flame retardants are generally incorporated into the product (e.g., foam or textile) during the early stages of manufacturing. Additives are mixed throughout the formulation, but are not chemically bound. Therefore, these additives have a much higher potential to migrate, or leach, from the product into the environment under normal conditions.

Low Toxicity: Effects on several human health endpoints should be minimized. These effects include: cancer hazard, skin sensitization, reproductive effects, developmental effects, neurological effects, systemic effects and mutagenicity. Section 4 discusses methods to characterize these effects and presents results of the screening level evaluations for the 14 formulations assessed in this report.

5.2 Aesthetic and Performance Considerations

Scorching is a primary concern in the manufacture of flexible polyurethane foam in general, and is a particular concern for low-density foams. Light scorching results in discoloration or yellowing of the foam, while severe scorching can cause decomposition resulting in permanent damage to the foam. This phenomenon occurs because of the high temperatures that are generated during production of the foam bun.

Scorching is more prevalent in low-density foams because of the necessity to use toluene diisocyanate (TDI), which enables the foam to achieve low densities, better firmness and better support. Methyl diphenyl diisocyanate (MDI) is used to manufacture higher density foams as well as memory foams. The use of TDI causes a more exothermic (heat generating) reaction than the use of MDI. Therefore, a higher thermally resistant flame retardant is required for manufacturing low-density foams.

PentaBDE allows for the manufacture of low-density flame-retarded foam that is “snow white” in color. Because of its aesthetic desirability, it became the industry standard in mattresses and bedding products, as well as in many upholstered furniture applications. Greater acceptance of off-white foams could allow manufacturers to choose from a wider variety of alternative flame retardants. Barrier fabrics are allowing mattress manufacturers to mask the color of foam so that it will not be visible to the consumer. Other characteristics of foam that can be affected by the choice of flame retardants include firmness, durability and flexibility.

5.3 Process and Equipment Considerations

Another important consideration when selecting an alternative for pentaBDE is the feasibility of using the new chemical in an industrial setting. Ideally the alternative should be compatible with existing process equipment at foam manufacturing facilities. If it is not, the plants will be forced to modify their processes and potentially to purchase new equipment. The ideal alternative would be a drop-in replacement that has similar physical and chemical properties such that existing storage and transfer equipment as well as foam production equipment can be used without significant modifications.

For example, most U.S. foam facilities are equipped to store and process liquid flame-retardant formulations through pipes, metering systems and pumps. A solid alternative may require foam plants to make significant investments for conveyorized transfer, dust control systems and solid weighing apparatus. These modifications are feasible, from an engineering point of view, but may be cost prohibitive in certain circumstances.

Similarly, many foam "recipes" and manufacturing procedures are based on the addition of liquid flame-retardant chemicals. Addition of a solid flame retardant may require changes such as additional mixing steps and alteration of the process times. In some cases, these changes can have significant effects on foam quality or cost-effectiveness of manufacture.

5.4 Economic Viability

Foam manufacturing is a very competitive market in the United States and around the world. A flame-retardant alternative that is either more expensive per pound, or requires more flame retardant per linear foot to meet the fire safety standards will increase the foamer's raw material costs. In this situation, a foam manufacturer will attempt to pass the cost on to their customers (e.g., the furniture manufacturer), who will subsequently pass the cost to consumers. If this increase causes a significant market share loss, the foam manufacturer may not be able to compete and may be forced to discontinue use of the alternative, making the alternative economically unfeasible.

5.5 Alternatives Technologies (General)

Potential alternatives for pentaBDE can be separated into two categories: (1) alternative chemicals, and (2) alternative technologies. Chemical alternatives are the focus of this report; however this section provides a brief discussion of three currently-available alternative technologies being considered for further investigation by the Furniture Flame Retardancy Partnership: barrier technologies, graphite impregnated foam and surface treatment. Graphite impregnated foam and surface treatments have limited commercial uses; therefore, they are only briefly discussed. Barrier technologies are predominantly used in mattress manufacturing rather than residential upholstered furniture. However, there is considerable interest in future applications for furniture. Future partnership activities may focus on barrier technologies if appropriate.

In addition to the following technologies, it should be noted that some furniture designs exclude the use of filling materials, and even fabric altogether. Design therefore, should be considered when evaluating alternative means for achieving flame retardancy in furniture.

5.5.1 Barrier Technologies

Flame-retardant barrier materials can be a primary defense in protecting padding for furniture and mattresses. Manufacturers can layer barrier materials to improve the flame retardancy of their products. This layering approach allows a product to maintain its fire resistance even if one layer is compromised.

There are many types of barrier materials available. Fabrics composed of natural fibers such as cotton that are chemically treated to make them flame retardant are flame-retardant barrier materials. The hazards of these chemical treatments have not been assessed in this report. Fabrics composed of synthetic fibers that are inherently flame retardant are also flame-retardant barrier materials. Plastic films derived from flame-retardant resins are also flame-retardant barrier materials. These materials are designed and manufactured to meet specific flammability standards. This also explains the large number of flame-retardant barrier materials that are available. Flame-retardant barrier materials can be characterized by cost, resulting in three primary groups.

The first group of flame-retardant materials is the chemically treated, primarily boric acid treated, cotton-based materials. These materials are the least expensive flame-retardant barrier materials available. Mattress manufacturers that base their material decisions predominantly on cost prefer these flame retardants.

The second group of flame-retardant materials is a blend of inexpensive natural fibers and expensive synthetic fibers. Synthetic fibers used in these blends include VISIL, Basofil, Polybenzimidazole, KEVLAR, NOMEX and fiberglass. Smaller manufacturers of furniture and mattresses in niche markets use these materials. These blends are commonly used in bus and airplane seating.

The third group of flame-retardant materials is composed solely of expensive, high-performance synthetic fibers. They are generally used in industrial or high-performance applications such as firemen's coats and astronaut space suits.

Barrier materials can also be divided into woven or nonwoven fabrics. Woven fabrics tend to use general weaving technology to manufacture the fabrics. Manufacturers can customize fabrics to meet specific customer needs. Nonwoven fabrics are created using quite different technologies. Thermally bonded fabrics are a type of nonwoven fabrics. These materials consist of a core, typically cotton, which is fed with one or two outer layers of melt blown and/or spunbond polypropylene webs. The polypropylene web serves as the binder in this process. The core and the web pass between a smooth and a patterned calendar. The calendars are heated and thermally bind the core to the web. This process creates thermally bonded laminates. Another type of nonwoven fabrics is needle-punched nonwovens. In this process, a spun bonded or carded web passes under a needle board that contains thousands of needles. As the needle passes into the web, a barb catches a fiber and passes it through the web, interlocking the fibers.

One unique group of barrier materials is flame-retardant films. The films do not have the strength or texture to be used as an external barrier. The film can be used to wrap the foam cushions or it can be quilted with flame-retardant fabrics for added support and an extra layer of fire protection. Neoprene film is a common flame-retardant film. One type of material that competes with neoprene film is fiberglass fabric.

Mattress and barrier manufacturers are now using barrier technology to meet new fire safety standards in the state of California (California Technical Bulletins 603 and 604). Flame-retardant cotton batting can be used in mattresses to provide cushion while reducing the amount of foam that is needed.

5.5.2 Graphite Impregnated Foams

Graphite impregnated foam (GIF) can be considered an "inherently flame-resistant foam" that is self-extinguishing and highly resistant to combustion. It is a relatively new technology and is largely used in niche markets such as for general aircraft seating. GIF technology produces foam that can meet airline fire safety standards for the seats with a reduced dependency on flame-retarded fabric. By minimizing the expense associated with flame-retardant fabric, GIF modified foams can be priced competitively.

GIF technology reportedly allows the design and fabrication of complex, comfortable and aesthetically pleasing seating for private aircraft. While GIF foam seating promises the possibility of eliminating the need for barrier fabrics, there are tradeoffs. When the barrier is removed, comprehensive composite flammability testing will be required on each new seat design to meet current fire safety standards (Federal Airways Regulation Part 25 Appendix F).

5.5.3 Surface Treatments

Surface treatments are also used in some applications and niche markets and may be appropriate for some textile manufacturing and furniture manufacturing readers of this document. However, surface treatments may not be viable as industry-wide replacements for pentaBDE for use in low-density foam for the following reasons:

There have been many proposals to achieve good resistance to ignition by post impregnation of foam with a variety of additives including borates, phosphates, various ammonium salts, etc.
In addition to durability concerns (many surface treatments wash off or degrade over time), there are other considerations that limit their use.

The main concern is difficulty in achieving uniform impregnation of a foam cushion, which may be 5 or 6 inches thick. In addition, many of these systems are water-based and the impregnated pieces then have to be dried, which is a slow and expensive process. The drying process also tends to produce a thin crust of the additive on the surface of the flexible polyurethane foam cushion. A variation of this approach has been to surface treat the finished upholstered cushion. This process must occur at the furniture assembly plants, which are not typically equipped for chemical processing. Some surface treatments can also leave an undesirable coating on the fabric cover or the cushion that is subject to disruption by friction during use.

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Appendix A

PentaBDE Facts

Summary of USEPA's Understanding of PBDEs

Polybrominated diphenylethers (PBDEs) are members of a broader class of brominated chemicals used as flame retardants; these are called brominated flame retardants, or BFRs. There are commercial mixtures of PBDEs with different average amounts of bromination: penta-, octa-, and decaBDE. These chemicals are major components of commercial formulations often used as fire retardants in furniture foam (pentaBDE), plastics for TV cabinets, consumer electronics, wire insulation, backcoatings for draperies and upholstery (decaBDE) and plastics for personal computers and small appliances (octaBDE). The value of these chemicals is their ability to slow ignition and rate of fire growth, and as a result increase available escape time in the event of a fire involving the above consumer products.

Although use of these chemicals is intended to save lives and property, there have been unintended consequences. Environmental monitoring programs in Europe, Asia, North America, and the Arctic have detected several PBDEs in human breast milk, fish, aquatic birds and elsewhere in the environment. Tetra- to hexabrominated diphenyl ethers are the PBDEs most frequently detected in wildlife and humans. The exact mechanisms or pathways by which the PBDEs end up in the environment and humans are not known yet, but would include releases from manufacturing or processing of the chemicals into products like plastics or textiles, aging and wear of the end consumer products and direct exposure during use (e.g., from furniture).

EPA is not only interested in responding to monitoring data, however. The Agency continually looks for pollution prevention opportunities; the Pollution Prevention Act of 1990 and EPA's Pollution Prevention Strategy establish that pollution should be prevented or reduced at the source whenever feasible. The Agency has also made protection of children's health a fundamental goal of public health and environmental protection in the United States.

In general, the human health and environmental concerns are higher for the lower brominated mixtures (i.e., pentaBDE and octaBDE), and data suggest that higher brominated forms such as decaBDE can be altered to form more toxicologically active lower brominated forms. The limited toxicity test data that is currently available indicate the potential for adverse effects to humans and environmental organisms, especially for lower brominated mixtures, but existing hazard and exposure information on PBDEs is incomplete. More needs to be understood about the environmental fate and the exposure pathways that lead to PBDE presence in wildlife and people. PBDEs appear to be persistent and bioaccumulative in the environment. EPA believes an improved understanding of potential risks posed by the different PBDE mixtures in their various use applications is needed. EPA is addressing PBDE information needs with a three-pronged approach, which includes:

- Efforts to better understand the environmental properties, exposure pathways and how these chemicals are getting into human tissue;
- Research and detailed testing to determine health and environmental effects; and
- Evaluation of potential substitutes, which includes the analysis of technical performance, cost-effectiveness and risk-risk trade-offs related to fire prevention and toxicity.

EPA offices and regions are working with fire safety advocates, industry, environmental and public health groups, other federal agencies, state governments and other national governments to answer the key questions and provide a basis for informed risk reduction decisions, including potential regulatory and voluntary actions. In November 2003, Great Lakes Chemical Corp., the only U.S. manufacturer of pentaBDE and octaBDE, announced a voluntary phase out of both those chemicals by the end of 2004.

Toxicity

There are commercial mixtures of PBDEs with different average amounts of bromination: penta-, octa- and decaBDE. In general, the human health and environmental concerns are greater for the lower brominated mixtures.

<u>Penta- and OctaBDE</u>

Effects on induction of hepatic enzymes were the basis of the EPA Integrated Risk Information System (IRIS) assessments of commercial pentaBDE and octaBDE mixtures which were completed in 1990. However, although liver enzyme induction was used as the basis for the RfD then, based on current methodology, this endpoint would not now be used as the basis of an RfD given the absence of other negative liver effects or histopathology. An update of the IRIS assessment for PBDE's is in progress. Several recent studies in young laboratory animals (rats and mice) exposed to commercial pentaBDE or to several individual congeners during gestation have shown some evidence of alterations in several behavioral parameters, deficits in learning and memory, and delays in the onset of puberty. Prenatal exposure to octaBDE mixtures in laboratory animals has resulted in reductions in fetal body weight, and delays in ossification - a longer than normal period before hardening of the bones. PentaBDE and octaBDE mixtures and individual congeners have also been shown to disrupt normal thyroid hormone levels in adult rats and mice. This could have possible concerns for developmental neurotoxic effects since it is well-established that disruption of thyroid hormone levels in the pregnant female may affect brain development in the fetus. The National Toxicology Program (an interagency program consisting of relevant toxicology activities of the Centers for Disease Control, Food and Drug Administration and National Institutes of Health) plans to conduct both chronic and subchronic toxicity studies on the commercial pentaBDE mixture, as well as the individual congeners appearing in greatest concentration in the mixture.

<u>DecaBDE</u>

Less is known about the potential toxicity of decaBDE. However, in contrast to penta- and octaBDE, decaBDE is poorly absorbed which may limit its potential toxicity. Some studies have shown thyroid and liver toxicity. Prenatal developmental toxicity studies in animals have been equivocal. A recent study in mice has provided some evidence of behavioral alterations. The European Commission will be requiring a more complete developmental neurotoxicity study in rodents to help clarify the potential for decaBDE exposure to result in developmental neurotoxicity. In addition, exposure to very high doses of decaBDE has been shown to cause tumors in laboratory animals.

Exposure

PBDEs have been measured in breast milk, adipose tissue and blood serum from human populations in Sweden, Finland, Germany, Japan, Spain, Canada and the United States. PBDE concentrations have steadily increased over 20 years of monitoring conducted in Sweden and Germany. In Sweden, PBDE levels in breast milk had doubled every 5 years between 1972 and 1997, with a decreasing trend since 1997. North American data are limited and additional studies are ongoing to determine relative levels in breast milk and blood serum compared to those found in Europe. However, average levels as measured in 23 human adipose tissue samples and 32 serum samples from among California women and 50 breast milk samples from Canada were higher than PBDE levels measured in Sweden.

Limited monitoring studies have found PBDEs in air, water, sediment, biota and sewage sludge throughout North America. The highest concentrations are generally associated with locations near facilities manufacturing or processing PBDEs. Concentrations of PBDEs are higher in municipal sewage sludge than in other environmental media. Recently reported PBDE concentrations in the United States and Canada are greater than those reported in Europe and Asia.

Different congeners are found at different levels in environmental media and wildlife. Generally the highest measured concentrations are for the tetra (>50%), penta (20-30%), hexa (15-20%) and hepta and octa brominated (< 20%) congeners. Which congeners are found and their relative and absolute concentrations vary from site to site.

Questions and Answers on PBDEs

1. What are PBDEs?

Polybrominated diphenylethers (PBDEs) are members of a broader class of brominated chemicals used as flame retardants; these are called brominated flame retardants, or BFRs. There are three commercial mixtures of PBDEs with differing average amounts of bromination: penta-, octa-, and decaBDE.

2. What are PBDEs used for?

These chemicals are major components of commercial formulations often used as flame retardants in furniture foam (pentaBDE), plastics for TV cabinets, consumer electronics, wire insulation, and backcoatings for draperies and upholstery (decaBDE), and plastics for personal computers and small appliances (octaBDE). The benefit of these chemicals is their ability to slow ignition and rate of fire growth, and as a result increase available escape time in the event of a fire.

3. What are concerns associated with PBDEs?

Although use of flame retardants saves lives and property, there have been unintended consequences. There is growing evidence that PBDEs persist in the environment and accumulate in living organisms, as well as toxicological testing that indicates these chemicals may cause liver toxicity, thyroid toxicity, and neurodevelopmental toxicity. Environmental monitoring programs in Europe, Asia, North America, and the Arctic have found traces of several PBDEs in human breast milk, fish, aquatic birds, and elsewhere in the environment. Particular congeners , tetra- to hexabrominated diphenyl ethers, are the forms most frequently detected in wildlife and humans. The mechanisms or pathways through which PBDEs get into the environment and humans are not known yet, but could include releases from manufacturing or processing of the chemicals into products like plastics or textiles, aging and wear of the end consumer products, and direct exposure during use (e.g., from furniture).

4. What is the Agency doing to better understand the possible risks from exposure to PBDEs?

EPA is currently evaluating a risk assessment and data needs analysis on PBDEs that was developed by industry for the Voluntary Children's Chemical Evaluation Program (VCCEP). This assessment evaluates the potential risks to children and prospective parents from all potential exposure scenarios. EPA will be releasing its views of the assessment, including any further VCCEP data needs, in the next few months.

Directly or through grant mechanisms, EPA has been supporting research aimed at a range of topics related to PBDEs, including measuring PBDE levels in umbilical cord blood from newborn U.S. infants, mothers' blood, house dust, food, breast milk, and children; potential thyroid toxicity and developmental neurotoxicity; and the environmental fate of the PBDEs upon their release during production or after disposal of products that contain these chemicals.

EPA's Office of Research and Development, National Center for Environmental Assessment, is enhancing its Integrated Risk Information System (IRIS) database on the PBDEs. IRIS is a database of human health effects that may result from exposure to substances found in the environment. The Agency developed IRIS to provide consistent information on chemical substances for use in risk assessments, decision-making and regulatory activities. The information in IRIS is intended for those without extensive training in toxicology, but with some knowledge of health sciences.

5. How does this action complement the decision by the sole US manufacturer to phase out production by December 31, 2004?

This action builds on the November 3, 2003, announcement by the Great Lakes Chemical Corporation, the only U.S. manufacturer of these chemicals, who agreed to voluntarily phase-out production by December 31, 2004. In 2003, EPA commended Great Lakes Chemical Corporation for taking this responsible action. EPA is concerned that manufacture or import could be reinstated in the future, and thus believes it is necessary to have the opportunity to evaluate any new manufacture or import associated with these chemicals.

6. Why are these chemical important and are there substitutes?

These chemicals provide a very important benefit because of their ability to save lives and property by slowing ignition and rate of fire growth, and therefore increase available escape time in the event of a fire. However, EPA also believes both the phase out and the Significant New Use rule will further spur the development of safer alternatives.

EPA has been working to ensure that following the phasing out of these two chemicals, acceptable alternatives are available to industry. Such alternatives would need to meet technological requirements of industry users, flame retardancy requirements in US standards, and present lower hazards than the chemicals for which they are substituting. To promote these goals and to explore the safety of alternative flame retardant chemicals, EPA has convened a group of stakeholders in its Furniture Flame Retardancy Partnership, including chemical manufacturers and users, the furniture industry, government agencies, and consumer groups, who will work together to evaluate possible alternatives to PentaBDE.

7. Should consumers discard any products that might contain PentaBDE or Octa?

No, the EPA does not believe that there is a need to remove or replace products that may contain these chemicals. EPA has not concluded that PBDEs pose an unreasonable risk to human health or the environment. However, due to growing concerns, EPA believes that the phase out and the regulatory action taken in this announcement are useful steps to minimize and ultimately help prevent further exposure to these chemicals.

8. What are PBDEs commonly used for?

The PBDEs are major components of commercial formulations often used as fire retardants in furniture foam, plastics for TV cabinets, consumer electronics, wire insulation, and back-coatings for draperies and upholstery, and plastics for personal computers and small appliances. These chemicals slow ignition and rate of fire growth, and, as a result, increase available escape time in the event of a fire involving the above consumer products.

9. How are people exposed to PBDEs?

PBDEs are not chemically bound to plastics, foam, fabrics, or other products in which they are used, making them more likely to leach out of these products. PBDEs may enter the air, water and soil during their manufacture and use in consumer products. The primary route of human exposure is currently unclear.

10. What is the Agency doing to better understand the occurrence of PBDEs in the environment?

EPA is addressing PBDE information needs with a three-pronged approach which includes: 1) efforts to better understand the environmental properties, exposure pathways, and how these chemicals are getting into human tissue; 2) research and detailed testing to determine health and environmental effects from exposure to PBDEs; and 3) evaluation of potential PBDE substitutes, which includes the analysis of technical performance, cost-effectiveness, and risk-risk trade-offs related to fire prevention and toxicity.

11. What efforts are underway to discourage continued use of the PBDEs?

In November 2003, the Great Lakes Chemical Corporation announced a voluntary phase out of PentaBDE and OctaBDE by the end of 2004. Great Lakes is the only U.S. manufacturer of these PBDEs. To follow up on this voluntary action, EPA is working with chemical manufacturers and end users to facilitate an orderly transition to safer substitutes. The State of California has enacted a law banning use of PentaBDE and OctaBDE by January 2008 (recently changed to June 1, 2006) and other states (including Maine, Hawaii, Washington, and New York) are also considering or have passed similar legislation. In Europe, the European Union enacted a ban on PentaBDE and OctaBDE in all products which took effect on August 15, 2004.

EPA is also working with the fire safety advocates, chemical manufacturers, manufacturers of end products such as furniture or plastics for electronics, environmental and public health groups, other federal agencies, state governments, and other nations to answer key questions and help people make informed decisions based on risk. EPA is considering both regulatory and voluntary actions.

Appendix B

Interpretive Guidance

Interpretive Guidance Document for Sustainable Futures Summary Assessment
Updated September 2004

This document was developed to help interpret results from the Sustainable Futures / P2 Framework models. Information is also included here which helps assign concern levels to results based on criteria from U.S. EPA OPPT's New Chemicals Program http://www.epa.gov/oppt/newchems/index.htm. Information contained in this document is presented in greater detail in the P2 Framework Manual. For more information on the models, estimations provided, and interpretation of results, please check the manual, which can be downloaded from http://www.epa.gov/oppt/p2framework/docs/p2manua.htm.

Model Availability

- EPISuite™ - download at no cost from http://www.epa.gov/opptintr/exposure/docs/episuite.htm
- ECOSAR - download at no cost from http://www.epa.gov/oppt/newchems/21ecosar.htm
- PBT Profiler - use on-line at no cost at www.pbtprofiler.net
- Cancer Expert System / OncoLogic - contact Bill Waugh, waugh.bill@epa.gov for information. U.S. EPA has purchased the commercial rights to OncoLogic and plans to make the model publicly available.
- E-FAST - download at no cost from http://www.epa.gov/opptintr/exposure/docs/efast.htm
- ChemSTEER - download at no cost from http://www.epa.gov/opptintr/exposure/docs/chemsteer.htm

Physical/Chemical Properties and Environmental Fate Estimations

EPISuite™ - Entering Data

The chemical structure can be entered using SMILES notation - or - if the chemical has a CAS Registry Number, the CAS numbers may be entered and the structure will be retrieved from the EPISuite™ built-in database if available. There is also a name lookup function that allows the user to retrieve chemical information without knowing the chemical structure or CAS number.

If any experimental data are available for the chemical, then all data should be entered into the input screen for EPISuite™.

For chemicals that are known liquids with no experimental MP data, enter 20 deg C as an experimental MP into the input screen for all EPISuite™ predictions.

Interpreting Results from EPISuite™

Melting Point and Boiling Point - Estimated by MPBPWIN
MP < 25 deg C = Liquid MP > 25 deg C = Solid BP < 25 deg C = Gas

Vapor Pressure - Estimated by MPBPWIN
$\geq 10^{-4}$ = Vapor (gas) phase 10^{-5} - 10^{-7} = Vapor and particulate phase $\leq 10^{-8}$ = Solid phase
For chemicals with a VP < 10^{-6}, there is low concern for inhalation exposure.

Water Solubility (mg/L) - Estimated by WSKOWWIN

> 10,000	Very soluble
> 1,000 - 10,000	Soluble
> 100 - 1,000	Moderate solubility
> 0.1 - 100	Slightly soluble
< 0.1	Insoluble

Log K_{ow} (Log P) - Estimated by KOWWIN

< 1	Highly soluble in water (hydrophilic)
> 4	Not very soluble in water (hydrophobic)
> 8	Not readily bioavailable
> 10	Not bioavailable - difficult to measure experimentally

Henry's Law Constant (atm-m^3/mole) - Estimated by HENRYWIN

$\geq 10^{-1}$	Very volatile from water
10^{-1} - 10^{-3}	Volatile from water
10^{-3} - 10^{-5}	Moderately volatile from water
10^{-5} - 10^{-7}	Slightly volatile from water
< 10^{-7}	Nonvolatile

If experimental vapor pressure ***and*** water solubility data are available and entered as input data into EPISuite™, then the VP/Wsol estimate (instead of the bond or group estimation method) should be used.

Atmospheric Oxidation Half-life - Estimated by AOPWIN

≤ 2 hours	Rapid
2 hrs - ≤ 1 day	Moderate
> 1 day - ≤ 10 days	Slow
>10 days	Negligible
>2 days	Has potential for long range transport in air

Hydrolysis Rates - Estimated by HYDROWIN
- Only Esters, Carbamates, Epoxides, Halomethanes, and certain Alkyl Halides are estimated in HYDROWIN.

Biodegradation - Estimated by BIOWIN: 3 Models available in EPISuite™

1. Probability of Rapid Biodegradation (BIOWIN):

BIOWIN Linear and BIOWIN Nonlinear

> 0.50 Likely to biodegrade fast

< 0.50 *Not* likely to biodegrade fast

2. Expert Survey Biodegradation (Primary/Ultimate):

Calculated Rating	Time Required for Biodegradation
5.0	Hours
4.5	Hours - days
4.0	Days
3.5	Days - weeks

Predicted Rating	Time Required for Biodegradation
5.0	Hours
4.0	Days
3.0	Weeks
2.5	Weeks - months
2.0	Months
1.0	Longer

3. Ready Biodegradability Model (MITI):

MITI Linear and MITI Nonlinear

> 0.50 Ready Biodegradable

< 0.50 Not Ready Biodegradable

Soil Adsorption Coefficient (Log K_{oc}) - Estimated by PCKOCWIN

≥ 4.5	Very strong sorption to soil and sediment, negligible migration potential to groundwater
3.5 - 4.4	Strong sorption to soil and sediment, negligible to slow migration potential to groundwater
2.5 - 3.4	Moderate sorption to soil and sediment, slow migration potential to groundwater
1.5 - 2.4	Low sorption to soil and sediment, moderate migration potential to groundwater
< 1.5	Negligible sorption to soil and sediment, rapid migration potential to groundwater

Bioconcentration Factors - Estimated by BCFWIN

> 5000	High bioconcentration potential
1000 - 5000	Moderate bioconcentration potential
< 1000	Low bioconcentration potential

STPWIN - Percent Removal in Sewage Treatment Plants

– Gives an indication of the percent removed from biodegradation (Bio P), sludge adsorption (Bio S), and aeration (Bio A) in a POTW or Sewage Treatment Plant.

– Negligible biodegradation (half-life = 10,000 hours) is the default value for the primary clarifier (P), aeration vessel (A), and final settling tank (S) unless otherwise specified in the input screen for EPISuite™. If data are available for the chemical, these half-lives can be changed in the input screen using the following guidance:

  1 hour = for chemicals with data suggesting *rapid* biodegradation potential
  3 hours = for chemicals with data suggesting *moderate* biodegradation potential
  30 hours = for chemicals with data showing *slow* biodegradation potential
  10,000 hours = default rate for chemical with *unknown* biodegradation potential

LEV3EPI - Fugacity Model

– Provides an indication of which environmental compartment the chemical is expected to partition to and calculates an approximate persistence time.

WVOL - Volatilization from Water

– Uses molecular weight, Henry's Law Constant, and water solubility to estimate an ***upper*** limit for volatilization from a body of water. The model ***does not*** take into account potential adsorption to sediment and suspended organic matter when the K_{oc} is high, which can increase the volatilization half-life dramatically. Therefore, if the K_{oc} for a given chemical is high, the volatilization half-lives for a model river and model lake are expected to be significantly higher than predicted in WVOL.

Persistence

U.S. EPA describes Persistence criteria in the PBT category for Premanufacture Notices in the Category for Persistent, Bioaccumulative, and Toxic New Chemical Substances at http://www.epa.gov/tri/pbt-final_rule.pdfhttp://www.epa.gov/fedrgstr/EPA-TOX/1999/November/Day-04/t28888.htm and in the final rule for TRI reporting of PBT Chemicals http://www.epa.gov/tri/pbt-final_rule.pdf. These criteria are used by the PBT Profiler (described in this document) to estimate environmental persistence potential of chemicals. These Persistence criteria are:

PERSISTENCE	Not Persistent	Persistent	
Water, Soil, Sediment*	< 60 d	. 60 d	> 180 d
Air**	. 2 d	> 2 d	

* New Chemical Program Criteria
** TRI Reporting Criteria

Hazard Estimations

Aquatic Toxicity Hazard - ECOSAR

Develop Full Standard Aquatic Toxicity Profile
The standard aquatic toxicity profile consists of 3 acute values (fish LC_{50}, daphnid LC_{50}, and algae EC_{50}) and 3 chronic values (fish ChV, daphnid ChV, and algae ChV). Examples of toxicity values that are generally used to fulfill the standard aquatic toxicity profile are provided below.

Organism	Acute Toxicity Values	Chronic Toxicity Values
Fish	96-hour LC_{50}	30-day ChV
Daphnid (Aquatic Invertebrate)	48-hour LC_{50}	ChV or 16-day EC_{50}
Algae	72- or 96-hour EC_{50}	ChV

A full standard profile for each chemical should be created using either predicted or experimental data. If no predicted or experimental data are available for the chemical of interest, then analog data may be used. If a single measured or predicted toxicity value is available for a species but the corresponding acute or chronic value is not, then an acute to chronic ratio (ACR) can be used to estimate the corresponding acute or chronic toxicity value:

Chronic toxicity estimate = (acute toxicity value) / (ACR)
Acute toxicity estimate = (chronic toxicity value) x (ACR)

An ACR of 10 is commonly applied to fish and daphnids and an ACR of 4 is commonly applied to algae. Example calculations are provided below.

Fish LC_{50} = 0.10 mg/L → extrapolated fish ChV = (0.10 mg/L)/10 = 0.01 mg/L (ppm)
Algae ChV = 0.02 mg/L → extrapolated algae EC_{50} = (0.02 mg/L) x 4 = 0.08 mg/L (ppm)

A full toxicity profile needs to be developed to perform an aquatic toxicity assessment. If an acute or chronic toxicity endpoint cannot be determined for one or more species from measured data on the chemical or analog or from predicted data, then category data can be used to fulfill the endpoint. For example, a fish or daphnid toxicity value can be estimated using the fish-to-daphnid toxicity ratio of chemicals within the same category (e.g., acrylates). Use data from multiple chemicals if possible. All assumptions and toxicity data used for the estimation need to be documented in the Sustainable Futures Summary Assessment.

The following guidance can be used to assign aquatic toxicity concern levels:

SF Concern	ECOSAR Results
Low	All 3 acute values are >100 mg/L, AND all three chronic values are >10.0 mg/L, or there are No Effects at Saturation (NES). *NES occurs when a chemical is not soluble enough to reach the effect concentration, i.e., the water solubility is lower than an effect concentration, or, for liquids, when K_{ow} criteria are exceeded for an endpoint. For solids, NES is expected if K_{ow} exceeds the specific SAR K_{ow} cutoffs, or the effect concentration is more than one order of magnitude ($\geq$10 X) less than water solubility.*
Moderate	Any of the 3 acute values are >1.0 mg/L and <100 mg/L, OR any of the chronic values are >0.1 mg/L and <10.0 mg/L
High	Any of the 3 acute values are <1.0 mg/L, OR any of the chronic values are <0.1 mg/L (except for substances with very low solubility (NES))

NOTE: K_{ow} cutoffs are specific to each SAR used in ECOSAR. The criteria can be found on the bottom of the results screen for ECOSAR or in the ECOSAR User's Manual available for download at http://www.epa.gov/oppt/newchems/sarman.pdf.

NOTE: Guidance on the evaluation of polymers can be found in
Boethling R.S. and J. V. Nabholz. 1997. "Environmental assessment of polymers under the U.S. Toxic Substances Control Act". *In:* Hamilton, J.D. and R. Sutcliffe, eds. Ecological assessment of polymers: Strategies for product stewardship and regulatory programs. New York, NY: Van Nostrand Reinhold, 187-234. ISBN 0-442-02328-6.

Human Health Hazard - Cancer - OncoLogic

Interpretation of OncoLogic Results:

SF Concern	OncoLogic Results	Definition - OncoLogic Result
Low	Low	Unlikely to be a carcinogen
Further Research Needed	Marginal	Likely to have equivocal carcinogenic activity
Moderate	Low-Moderate	Likely to be weakly carcinogenic
	Moderate	Likely to be moderately active carcinogen
High	Moderate-High	Highly likely to be a moderately active carcinogen
	High	Highly likely to be a potent carcinogen

Interpretation of Experimental Data:

SF Concern	Definition - Experimental Data
Low	Negative experimental data
Moderate	Positive cancer bioassay in experimental animals ***or*** chemical class known to produce carcinogenic effects
High	Positive experimental data in humans (e.g. epidemiology study)

NOTE: Measured data from a properly conducted study on the SF chemical or a relevant analog always takes precedence over predicted data.

Human Health Hazard - Non-Cancer

Criteria for Assigning Non-Cancer Hazard Concern Levels:

SF Concern	Definition - Experimental Data
Low	No concern identified
Moderate	Suggestive animal studies for chemical or analog(s) ***or*** chemical class known to produce toxicity
High	Evidence of adverse effects in humans ***or*** conclusive evidence of severe effects in animal studies

NOTE: Regulatory decisions will be made based on the following human health effects: reproductive; immune; developmental; neurotoxicity; and systemic.

NOTE: Guidance on the evaluation of non-cancer human health concerns of polymers can be found in: P2 Framework Manual, Oct 2003 version, edited Jan 2004, pg. 169-170 at: http://www.epa.gov/oppt/p2framework/docs/p2manua.htm

PBT Potential Estimation

PBT Profiler - U.S. EPA describes Persistence, Bioaccumulative, and Toxicity (PBT) criteria in the PBT category for Premanufacture Notices in the Category for Persistent, Bioaccumulative, and Toxic New Chemical Substances at http://www.epa.gov/fedrgstr/EPA-TOX/1999/November/Day-04/t28888.htm and in the final rule for TRI reporting of PBT Chemicals http://www.epa.gov/tri/pbt-final_rule.pdf. These criteria are used by the PBT Profiler to estimate PBT potential of chemicals.
These PBT criteria are:

PERSISTENCE	Not Persistent	Persistent	
Water, Soil, Sediment*	< 60 d	≥ 60 d	> 180 d
Air**	≤ 2 d	> 2 d	
BIOACCUMULATION	Not Bioaccumulative	Bioaccumulative	
Fish BCF*	< 1000	≥ 1000	≥ 5000
TOXICITY	Not Toxic	Toxic	
Fish ChV*	> 10 mg/L *or* No Effects at Saturation	0.1-10 mg/L	< 0.1 mg/L

NOTE: The PBT Profiler is not appropriate for certain types of chemicals, such as metals. Before using the PBT Profiler determine if the chemical being evaluated is appropriate for running in the PBT Profiler. Extensive information is provided within the on-line model at www.pbtprofiler.net
* New Chemical Program Criteria
** TRI Reporting Criteria

IMPORTANT NOTE:
Evaluate exposure if a moderate or high hazard concern has been identified for *any* endpoint.

Exposure Estimations

Aquatic Exposure - E-FAST

Predicted Environmental Concentration (PEC):
Amount expected to be found in surface water after release from industrial processes; also called surface water concentration (SWC).

Estimated values can be determined using E-FAST and found under the General SIC Code Information tab in the results screen. The **10% percentile, 7Q10 stream concentrations (µg/L)** are used for an SF Assessment.

To run E-FAST you will need to determine a chronic **Concentration of Concern (COC)** based on the toxicity values derived in the Aquatic Toxicity section. The COC is one of the inputs for the E-FAST program and an explanation for the determination of a chronic COC can be found on the following page of this document.

Human Exposure - ChemSTEER and E-FAST

For Occupational Exposure Doses:
LADD, ADD, and APDR values will be estimated by **ChemSTEER**

For General Population Exposure Doses:
LADDpot, ADDpot, and ADRpot values will be estimated by **E-FAST.** The **10% percentile values (mg/kg/day)** are used for an SF Assessment.

Lifetime Average Daily Dose (LADD or LADDpot):
The predicted lifetime exposure used to determine cancer risk usually based on an average lifetime of 70 - 75 years and a working lifetime of 30 - 40 years.

Potential Average Daily Dose (ADD or ADDpot):
The predicted dose that represents potential chronic exposure based on a duration of repeated exposure usually approximating an average of 30 years.

Potential Acute Dose Rate (APDR or ADRpot):
The predicted acute dose rate that represents acute exposure usually based on a single 8 hour working day exposure duration.

NOTE: For the purposes of an SF Assessment, the defaults for average lifetime, body weight, exposure duration, and ingestion rate are pre-set in both ChemSTEER and E-FAST and should not be changed unless accurate data for these inputs are available.

Risk Estimations *Reminder:* RISK = HAZARD x EXPOSURE

For chemicals with an identified hazard concern, the potential exposure must be determined to make an assessment of risk. If a low concern for hazard is identified (hazard approx. = 0) or very low exposure is identified (exposure approx. = 0), then there is an inherently low concern for risk because of the mathematical relationship between hazard and exposure.

Estimating Aquatic Risk

Determine an Acute and Chronic Concentration of Concern (COC):
Concentration at which potential acute or chronic aquatic toxicity may be of concern for aquatic species. Calculate a COC for every species in the full profile.

Acute COC:
Acute COC for fish = LC_{50} / (5)
Acute COC for daphnia = EC_{50} / (5)
Acute COC for algae = EC_{50} / (4) **-OR-** If an **algae ChV** value exists, use that value as the acute COC and do not estimate the COC using an EC_{50} value divided by a factor.

If a NOEC value is available from an acute study for any species, that value can be used directly as the acute COC. (No assessment factor needed)

Chronic COC:
Chronic COC for fish = ChV / (10)
Chronic COC for daphnia = ChV / (10)
Chronic COC for algae = ChV / (10)
If a NOEC value is available from a chronic study for any species, that value can be used directly as the chronic COC. (No assessment factor needed)

Example calculations are provided below:

Fish LC_{50} = 0.10 mg/L → calculated Acute COC = (0.10 mg/L) /5 = 0.02 mg/L (ppm)
Daphnid ChV = 0.02 mg/L → calculated Chronic COC = (0.02 mg/L) /10 = 0.002 mg/L (ppm)

NOTE: All COCs are rounded up to 1 significant digit (e.g., a COC of 1.75 ppb is rounded up to 2 ppb). All COC values less than 1 ppb are rounded up to 1 ppb for assessments due to limitations in reliable analytical methods to test below 1 ppb should verification be needed.

No values less than 1 ppb (the realistic detection limit) should be reported!!

Estimating Acute Aquatic Risk

The potential for acute risk to aquatic organisms exists if the predicted environmental concentration (PEC) is greater than the acute concentration of concern (COC).

If Acute COC > PEC Low concern for risk If Acute COC < PEC Potential for risk

Estimating Chronic Aquatic Risk

The potential for chronic risk to aquatic organisms may exist if the COC is exceeded for 20 days or more per year. There will be instances that you will determine a chronic COC exceeds the PEC, but if it is not exceeded for 20 days or more per year, then there is low concern for risk. This is because although there is a potential for the concentration of the chemical in the water to reach levels exceeding the hazardous level, the levels are not exceeded for a sufficient duration of time to induce any chronic effects.

The 20-day criterion is derived from partial life-cycle tests (daphnid chronic and fish early life- stage tests) that typically range from 21 to 28 days in duration. Low concern for chronic risk exists if the COC is exceeded on fewer than 20 days per year.

E-FAST will predict how many days per year the (PEC) exceeds the (COC). The number of days the COC is exceeded can be found on the PDM SIC tab in the output screen of E-FAST.

Example Worksheet for Identification of Acute and Chronic Risk to Aquatic Organisms:

Acute Endpoint	Value	Factor	Acute COC	PEC	Risk?
Fish LC50	0.079 ppm	5	0.02 ppm	0.055 ppm	**Yes**
Daphnid LC50	0.11 ppm	5	0.02 ppm	0.055 ppm	**Yes**
Algae EC50	0.083 ppm	4	0.07* ppm	0.055 ppm	No

* Since an algae ChV value was available (see below), the ChV value was used as the algae acute COC.

E-FAST indicated that the PEC exceeds the COC for 9.4 days per year

Chronic Endpoint	Value	Factor	Chronic COC	PEC	Risk?
Fish ChV	0.018 ppm	10	0.002 ppm	0.055 ppm	**Yes**
Daphnid ChV	0.027 ppm	10	0.003 ppm	0.055 ppm	No
Algae ChV	0.067 ppm	10	0.007 ppm	0.055 ppm	No

Aquatic Risk Summary: There is potential for acute risk to the aquatic environment because the PEC is greater than the acute COC (for fish and daphnids). There is low concern for chronic risk because even though the PEC exceeds the chronic COC for fish, it is only exceeded for 9.4 days according to E-FAST and under EPA guidelines, this is not a sufficiently long enough duration to induce chronic effects.

Estimating Human Health Non-Cancer Risk

For the determination of risk to the human population from non-cancer human health effects, a quantitative value called the Margin of Exposure (MOE) is calculated. This margin is essentially the established safety buffer between the hazardous effects level (dose) and the predicted exposure dose. The EPA OPPT office utilizes margins of exposure that they believe are sufficiently protective of human health when assessing new chemicals. The calculated MOEs for each chemical are compared to the MOE criteria used by the OPPT office and the results are evaluated to determine the potential for risk. When referring to non-cancer effects, these margins of exposure or safety buffers must be at least 100X or 1000X protective of human health depending on the type of non-cancer data identified in the hazard assessment.

If hazard data for ANY of the non-cancer health effect endpoints have indicated a moderate or high hazard concern, then an MOE for EACH moderate/high concern endpoint should be determined! The lowest MOE value calculated from that group should be recorded for assessment purposes and will be used as the quantitative value to determine the potential overall risk to human health from non-cancer effects.

The lowest MOE will represent the worst-case scenario for the chemical and therefore, if the lowest MOE does not indicate a risk, then there is an assumed low potential for risk for all other endpoints which had mathematically larger MOE values.

However, if even one of the endpoints has a calculated MOE indicating the potential for risk, then overall the chemical should be flagged as having potential risks to human health. The subsequent pages give more in-depth guidance on the determination of MOE for acute and chronic risk from occupational exposure and from exposures to the general population.

The following table shows the human health non-cancer endpoints and the corresponding acute/chronic exposure values to use for calculation of an MOE:

Endpoint	Exposure dose used for MOE calc.
Single Dose Studies	
Acute Toxicity	ADRpot (acute)*
Repeated Dose Studies	
Irritation	Can not be used to determine MOE
Skin Sensitizer	Can not be used to determine MOE
Reproductive Effects	ADDpot (chronic)
Immune System Effect	ADDpot (chronic)
Developmental Toxicity	ADRpot (acute)
Genotoxicity	Can not be used to determine MOE
Mutagenicity	Can not be used to determine MOE
Neurotoxicity	ADDpot (chronic)
Systemic Effects	ADDpot (chronic)
* Acute risk is ONLY assessed for chemicals with an LD_{50} value < 50 mg/kg.	

Estimating Acute Risk to the General Population using an MOE:

NOTE: When the acute toxicity studies indicate LD_{50} values > 50 mg/kg for a chemical, there is no need to calculate a Margin of Exposure (MOE) for acute exposure and a low concern for acute risk is assumed.

There is a potential acute hazard concern for chemicals with an LD_{50} < 50 mg/kg. A MOE needs to be calculated and the potential for acute risk to the general population needs to be assessed when acute toxicity studies with LD_{50} values < 50 mg/kg have been identified.

Margin of Exposure (MOE) based on Acute Exposure:
Ratio of the identified effect level (LD_{50} value determined in health hazard section) to the estimated acute dose rate (predicted from E-FAST).
MOEacute = LD_{50} (mg/kg) / ADRpot (from E-FAST)
MOE < 1000 indicates potential for risk
MOE > 1000 indicates low concern for risk

Estimating Chronic Risk to General Population or to Workers using an MOE:

NOTE: Regulatory decisions will be made based on the following human health effects: reproductive; immune; developmental; neurotoxicity; and systemic.

Margin of Exposure (MOE) based on Chronic Exposure:
An MOE is the ratio of the No-Observed Adverse-Effect-Level (NOAEL) or the Lowest-Observed Adverse-Effect-Level (LOAEL) for the effect (determined in health hazard section) to the estimated exposure value (predicted from exposure models). If both a NOAEL and LOAEL are available, then the NOAEL value is used for calculation of the MOE.

MOE, Occupational = NOAEL or LOAEL(Non-Cancer) / APDR or ADD (from ChemSTEER)
MOE, General Population = NOAEL or LOAEL(Non-Cancer) /ADRpot or ADDpot (from E-FAST)

Human Health Risk Summary: There is a potential risk concern for chemicals with an MOE < 100 based on studies with NOAEL values and for chemicals with MOE < 1000 based on studies with only LOAEL values. The preference is to identify a NOAEL value and use that value for your MOE calculations. The average daily dose (ADD or ADDpot) is used to determine an MOE with one exception; an MOE for developmental toxicity is based on the acute dose rate (APDR or ADRpot).

For Calculation based on NOAEL:
MOE < 100 indicates potential for risk
MOE > 100 indicates low concern for risk

For Calculation based on LOAEL:
MOE < 1000 indicates potential for risk
MOE > 1000 indicates low concern for risk

For MOE values based on ***developmental toxicity data*** a body weight of 60 kg should be used as input when determining the exposure values (ADD, ADR, LADD) instead of the default of 70 kg because that particular endpoint is only assessed in females.

Example Worksheet for Identification of the Potential for Acute and Chronic Risk to Human Health based on a Non-Cancer MOE:

Population	Effect	NOAEL	LOAEL	Exposure	MOE
Occupational	Systemic	40 mg/kg-d	200 mg/kg-d	1.8×10^{-2} mg/kg-d ChemSTEER ADD	2222
	Neurotox	40 mg/kg-d	200 mg/kg-d	1.8×10^{-2} mg/kg-d ChemSTEER ADD	2222
General Population	Systemic	40 mg/kg-d	200 mg/kg-d	2.1×10^{-6} mg/kg-d E-FAST ADDpot	1.9×10^{7}
	Neurotox	40 mg/kg-d	200 mg/kg-d	2.1×10^{-6} mg/kg-d E-FAST ADDpot	1.9×10^{7}

The MOE used to evaluate Risk from Occupational Exposure = 2222
The MOE used to evaluate Risk from General Population Exposure = 1.9×10^{7}

Occupational Risk Summary: There is low concern for risk from occupational exposure or exposures to the general population because the MOE's are greater than 100 (based on studies with a NOAEL).

Estimating Human Health Cancer Risk

US EPA has purchased the public rights to OncoLogic, the Cancer Expert System, and plans to make it publicly available. When it becomes available information on interpreting results from that model will be included in this document.

General Overview for a Cancer Risk Assessment:

For Occupational Exposure Doses: LADD will be calculated by **ChemSTEER**

For General Population Exposure Doses: LADDpot will be calculated by **E-FAST**.

$$\text{Slope Factor} = \text{Slope Factor (mg/kg-day)}^{-1} \text{ (Calculated)}$$

A measure of individual's extra risk (increased likelihood) of developing cancer for each incremental increase in exposure to a chemical. It approximates the upper bound of the slope of the dose-response curve using the linearized multistage procedure at low doses. The calculation of a slope factor requires tools that are not provided in the P2 Framework but can downloaded from the web for free. The software package is called The Benchmark Dose Software (BMDS), can be found at: http://cfpub.epa.gov/ncea/

$$\text{Cancer Risk} = \text{LADD or LADDpot} \times \text{Slope Factor}$$

Generally, a cancer risk of $> 1 \times 10^{-6}$ (1 in 1,000,000) for the general population and $> 1 \times 10^{-5}$ (1 in 100,000) for worker exposure indicates the potential for risk.

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